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Practical Guide To Computer Simulations

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Chapter 7

Randomness and Statistics

In this chapter, we are concerned with statistics in a very broad sense. This involves generation of (pseudo) random data, display/plotting of data and the statistical analysis of simulation results.

Frequently, a simulation involves the explicit generation of random numbers, for instance, as auxiliary quantity for stochastic simulations. In this case it is obvious that the simulation results are random as well. Although there are many simulations which are explicitly not random, the resulting behavior of the simulated systems may appear also random, for example the motion of interacting gas atoms in a container. Hence, methods from statistical data analysis are necessary for almost all analysis of simulation results.

This chapter starts (Sec. 7.1) by an introduction to randomness and statistics. In Sec. 7.2 the generation of pseudo random numbers according to some given probability distribution is explained. Basic analysis of data, i.e., the calculation of mean, variance, histograms and corresponding error bars, is covered in Sec. 7.3. Next, in Sec. 7.4, it is shown how data can be represented graphically using suitable plotting tools, *gnuplot* and *xmgrace*. Hypothesis testing and how to measure or ensure independence of data is treated in Sec. 7.5. How to fit data to functions is explained in Sec. 7.6. In the concluding section, a special technique is outlined which allows to cope with the limitations of simulations due to finite system sizes.

Note that some examples are again presented using the C programming language. Nevertheless, there exist very powerful freely available programs like R [R], where many analysis (and plotting) tools are available as additional packages.

7.1 Introduction to probability

Here, a short introduction to concepts of probability and randomness is given. The presentation here should be concise concerning the subjects presented in this book. Nevertheless, more details, in particular proofs, examples and exercises,

can be found in standard textbooks [Dekking et al (2005), Lefebvre (2006)]. Here often a sloppy mathematical notation is used for brevity, e.g. instead of writing "a function $g : X \to Y$, $y = g(x)$", we often write simply "a function $g(x)$".

A *random experiment* is an experiment which is truly random (like radioactive decay or quantum mechanical processes) or at least unpredictable (like tossing a coin or predicting the position of a certain gas atom inside a container which holds a hot dense gas).

Definition The *sample space* Ω is a set of all possible outcomes of a random experiment.

For the coin example, the sample space is $\Omega = \{\text{head, tail}\}$. Note that a sample space can be in principle infinite, like the possible x positions of an atom in a container. With infinite precision of measurement we have $\Omega^{(x)} = [0, L_x]$, where the container shall be a box with linear extents L_x (L_y, L_z in the other directions, see below).

For a random experiment, one wants to know the probability that certain events occur. Note that for the position of an atom in a box, the probability to find the atom *precisely at* some x-coordinate $x \in \Omega^{(x)}$ is zero if one assumes that measurements result in real numbers with infinite precision. For this reason, one considers probabilities $P(A)$ of subsets $A \subset \Omega$ (in other words $A \in 2^\Omega$, 2^Ω being the *power set* which is the set of all subsets of Ω). Such a subset is called an *event*. Therefore $P(A)$ is the probability that the outcome of a random experiment is inside A, i.e. one of the elements of A. More formally:

Definition A *probability function* P is a function $P : 2^\Omega \longrightarrow [0, 1]$ with

$$P(\Omega) = 1 \tag{7.1}$$

and for each finite or infinite sequence $A_1, A_2, A_3, \ldots$ of mutual disjoint events ($A_i \cap A_j = \emptyset$ for $i \neq j$) we have

$$P(A_1 \cup A_2 \cup A_3 \cup \ldots) = P(A_1) + P(A_2) + P(A_3) + \ldots \tag{7.2}$$

For a fair coin, both sides would appear with the same probability, hence one has $P(\emptyset) = 0$, $P(\{\text{head}\}) = 0.5$, $P(\{\text{tail}\}) = 0.5$, $P(\{\text{head, tail}\}) = 1$. For the hot gas inside the container, we assume that no external forces act on the atoms. Then the atoms are distributed uniformly. Thus, when measuring the x position of an atom, the probability to find it inside the region $A = [x, x + \Delta x] \subset \Omega^{(x)}$ is $P(A) = \Delta x / L_x$.

The usual set operations applies to events. The *intersection* $A \cap B$ of two events is the event which contains elements that are both in A and B. Hence $P(A \cap B)$ is the probability that the outcome of an experiment is contained in both events A and B. The *complement* A^c of a set is the set of all elements of Ω which are not in A. Since A^c, A are disjoint and $A \cup A^c = \Omega$, we get from Eq. (7.2):

$$P(A^c) = 1 - P(A)\,. \tag{7.3}$$

Furthermore, one can show for two events $A, B \subset \Omega$:

$$P(A \cup B) = P(A) + P(B) - P(A \cap B) \tag{7.4}$$

Proof $P(A) = P(A \cap \Omega) = P(A \cap (B \cup B^c)) = P((A \cap B) \cup (A \cap B^c)) \overset{(7.2)}{=} P(A \cap B) + P(A \cap B^c)$. If we apply this for $A \cup B$ instead of A, we get $P(A \cup B) = P((A \cup B) \cap B) + P((A \cup B) \cap B^c)) = P(B) + P(A \cap B^c)$. Eliminating $P(A \cap B^c)$ from these two equations gives the desired result. □

Note that Eqs. (7.2) and (7.3) are special cases of this equation.

If a random experiment is repeated several times, the possible outcomes of the repeated experiment are tuples of outcomes of single experiments. Thus, if you throw the coin twice, the possible outcomes are (head,head), (head,tail), (tail,head), and (tail,tail). This means the sample space is a power of the single-experiment sample spaces. In general, it is also possible to combine different random experiments into one. Hence, for the general case, if k experiments with sample spaces $\Omega^{(1)}, \Omega^{(2)}, \ldots, \Omega^{(k)}$ are considered, the sample space of the combined experiment is $\Omega = \Omega^{(1)} \times \Omega^{(2)} \times \ldots \times \Omega^{(k)}$. For example, one can describe the measurement of the position of the atom in the hot gas as a combination of the three independent random experiments of measuring the x, y, and z coordinates, respectively.

If we assume that the different experiments are performed *independently*, then the total probability of an event for a combined random experiment is the product of the single-experiment probabilities: $P(A^{(1)}, A^{(2)}, \ldots, A^{(k)}) = P(A^{(1)})P(A^{(2)}) \ldots P(A^{(k)})$.

For tossing the fair coin twice, the probability of the outcome (head,tail) is $P(\{\text{(head,head)}\}) = P(\{\text{head}\})P(\{\text{head}\}) = 0.5 \cdot 0.5 = 0.25$. Similarly, for the experiment where all three coordinates of an atom inside the container are measured, one can write $P([x, x + \Delta x] \times [y, y + \Delta y] \times [z, z + \Delta z]) = P([x, x + \Delta x])P([y, y + \Delta y])P([z, z + \Delta z]) = (\Delta x/L_x)(\Delta y/L_y)(\Delta z/L_z) = \Delta x \Delta y \Delta z/(L_x L_y L_z)$.

Often one wants to calculate probabilities which are restricted to special events C among all events, hence relative or *conditioned* to C. For any other event A we have $P(C) = P((A \cup A^c) \cap C) = P(A \cap C) + P(A^c \cap C)$, which means $\frac{P(A \cap C)}{P(C)} + \frac{P(A^c \cap C)}{P(C)} = 1$. Since $P(A \cap C)$ is the probability of an outcome in A and C and because $P(C)$ is the probability of an outcome in C, the fraction $\frac{P(A \cap C)}{P(C)}$ gives the probability of an outcome A and C relative to C, i.e. the probability of event A given C, leading to the following

Definition The *probability of A under the condition C* is

$$P(A|C) = \frac{P(A \cap C)}{P(C)}\,. \tag{7.5}$$

As we have seen, we have the natural normalization $P(A|C) + P(A^c|C) = 1$. Rewriting Eq. (7.5) one obtains $P(A|C)P(C) = P(A \cap C)$. Therefore, the calculation of $P(A \cap C)$ can be decomposed into two parts, which are sometimes easier to obtain. By symmetry, we can also write $P(C|A)P(A) = P(A \cap C)$.

Combining this with Eq. (7.5), one obtains the famous *Bayes' rule*

$$P(C|A) = \frac{P(A|C)P(C)}{P(A)} \,. \tag{7.6}$$

This means one of the conditional probabilities $P(A|C)$ and $P(C|A)$ can be expressed via the other, which is sometimes useful if $P(A)$ and $P(C)$ are known. Note that the denominator in the Bayes' rule is sometimes written as $P(A) = P(A \cap (C \cup C^c)) = P(A \cap C) + P(A \cap C^c) = P(A|C)P(C) + P(A|C^c)P(C^c)$.

If an event A is *independent* of the condition C, its conditional probability should be the same as the unconditional probability, i.e., $P(A|C) = P(A)$. Using $P(A \cap C) = P(A|C)P(C)$ we get $P(A \cap C) = P(A)P(C)$, i.e., the probabilities of independent events have to be multiplied. This was used already above for random experiments, which are conducted as independent subexperiments.

So far, the outcomes of the random experiments can be anything like the sides of coins, sides of a dice, colors of the eyes of randomly chosen people or states of random systems. In mathematics, it is often easier to handle numbers instead of arbitrary objects. For this reason one can represent the outcomes of random experiments by numbers which are assigned via special functions:

Definition For a sample space Ω, a *random variable* is a function $X : \Omega \longrightarrow \mathbb{R}$. For example, one could use $X(\text{head})=1$ and $X(\text{tail}) = 0$. Hence, if one repeats the experiments k times independently, one would obtain the number of heads by $\sum_{i=1}^{k} X(\omega^{(i)})$, where $\omega^{(i)}$ is the outcome of the i'th experiment.

If one is interested only in the values of the random variable, the connection to the original sample space Ω is not important anymore. Consequently, one can consider random variables X as devices, which output a random number x each time a random experiment is performed. Note that random variables are usually denoted by upper-case letters, while the actual outcomes of random experiments are denoted by lower-case letters.

Using the concept of random variables, one deals only with numbers as outcomes of random experiments. This enables many tools from mathematics to be applied. In particular, one can combine random variables and functions to obtain new random variables. This means, in the simplest case, the following: First, one performs a random experiment, yielding a random outcome x. Next, for a given function g, $y = g(x)$ is calculated. Then, y is the final outcome of the random experiment. This is called a *transformation* $Y = g(X)$ of the random variable X. More generally, one can also define a random variable Y by combining *several* random variables $X^{(1)}, X^{(2)}, \ldots, X^{(k)}$ via a function $\tilde{g}$ such that

$$Y = \tilde{g}\left(X^{(1)}, X^{(2)}, \ldots, X^{(k)}\right) \,. \tag{7.7}$$

In practice, one would perform random experiments for the random variables $X^{(1)}, X^{(2)}, \ldots, X^{(k)}$, resulting in outcomes $x^{(1)}, x^{(2)}, \ldots, x^{(k)}$. The final number is obtained by calculating $y = \tilde{g}(x^{(1)}, x^{(2)}, \ldots, x^{(k)})$. A simple but the most important case is the linear combination of random variables $Y = \alpha_1 X^{(1)} + \alpha_2 X^{(2)} + \ldots + \alpha_k X^{(k)}$, which will be used below. For all examples

considered here, the random variables $X^{(1)}, X^{(2)}, \ldots, X^{(k)}$ have the same properties, which means that the same random experiment is repeated k times. Nevertheless, the most general description which allows for different random variables will be used here.

The behavior of a random variable is fully described by the probabilities of obtaining outcomes smaller or equal to a given parameter x:

Definition The *distribution function* of a random variable X is a function $F_X : \mathbb{R} \longrightarrow [0, 1]$ defined via

$$F_X(x) = P(X \leq x) \tag{7.8}$$

The index X is omitted if no confusion arises. Sometimes the distribution function is also named *cumulative* distribution function. One also says, the distribution function defines a *probability distribution*. Stating a random variable or stating the distribution function are fully equivalent methods to describe a random experiment.

For the fair coin, we have, see left of Fig. 7.1

$$F(x) = \begin{cases} 0 & x < 0 \\ 0.5 & 0 \leq x < 1 \\ 1 & x \geq 1 \end{cases} . \tag{7.9}$$

For measuring the x position of an atom in the uniformly distributed gas we obtain, see right of Fig. 7.1

$$F(x) = \begin{cases} 0 & x < 0 \\ x/L_x & 0 \leq x < L_x \\ 1 & x \geq L_x \end{cases} . \tag{7.10}$$

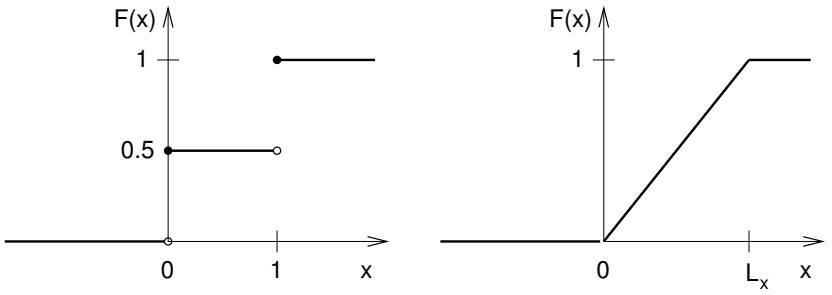


Figure 7.1: Distribution function of the random variable for a fair coin (left) and for the random x position of a gas atom inside a container of length L_x.

Since the outcomes of any random variable are finite, there are *no* possible outcomes $X \leq x$ in the limit $x \to -\infty$. Also, *all* possible outcomes fulfill $X \leq x$

for $x \to \infty$. Consequently, one obtains for all random variables $\lim_{x\to-\infty} F(x) = 0$ and $\lim_{x\to+\infty} F(x) = 1$. Furthermore, from Def. 7.1, one obtains immediately:

$$P(x_0 < X \leq x_1) = F_X(x_1) - F_X(x_0) \tag{7.11}$$

Therefore, one can calculate the probability to obtain a random number for any arbitrary interval, hence also for unions of intervals.

The distribution function, although it contains all information, is sometimes less convenient to handle, because it gives information about cumulative probabilities. It is more obvious to describe the outcomes of the random experiments directly. For this purpose, we have to distinguish between *discrete* random variables, where the number of possible outcomes is denumerable or even finite, and *continuous* random variables, where the possible outcomes are non-denumerable. The random variable describing the coin is discrete, while the position of an atom inside a container is continuous.

7.1.1 Discrete random variables

We first concentrate on discrete random variables. Here, an alternative but equivalent description to the distribution function is to state the probability for each possible outcome directly:

Definition For a discrete random variable X, the *probability mass function* (pmf) $p_X : \mathbb{R} \to [0, 1]$ is given by

$$p_X(x) = P(X = x)\,. \tag{7.12}$$

Again, the index X is omitted if no confusion arises. Since a discrete random variable describes only a denumerable number of outcomes, the probability mass function is zero almost everywhere. In the following, the outcomes x where $p_X(x) > 0$ are denoted by $\tilde{x}_i$. Since probabilities must sum up to one, see Eq. 7.1, one obtains $\sum_i p_X(\tilde{x}_i) = 1$. Sometimes we also write $p_i = p_X(\tilde{x}_i)$. The distribution funcion $F_X(x)$ is obtained from the pmf via summing up all probabilities of outcomes smaller or equal to x:

$$F_X(x) = \sum_{\tilde{x}_i \leq x} p_X(\tilde{x}_i) \tag{7.13}$$

For example, the pmf of the random variable arising from the fair coin Eq. (7.9) is given by $p(0) = 0.5$ and $p(1) = 0.5$ ($p(x) = 0$ elsewhere). The generalization to a possibly unfair coin, where the outcome "1" arises with probability p, leads to:

Definition The *Bernoulli distribution with parameter* p ($0 < p \leq 1$) describes a discrete random variable X with the following probability mass function

$$p_X(1) = p, \quad p_X(0) = 1 - p\,. \tag{7.14}$$

Performing a Bernoulli experiment means that one throws a generalized coin and records either "0" or "1" depending on whether one gets head or tail.

There are a couple of important characteristic quantities describing the pmf of a random variable. Next, we describe the most important ones for the discrete case:

Definition

- The *expectation value* is

$$\mu \equiv \mathrm{E}[X] = \sum_i \tilde{x}_i P(X = \tilde{x}_i) = \sum_i \tilde{x}_i p_X(\tilde{x}_i) \tag{7.15}$$

- The *variance* is

$$\sigma^2 \equiv \mathrm{Var}[X] = \mathrm{E}[(X - \mathrm{E}[X])^2] = \sum_i (\tilde{x}_i - \mathrm{E}[X])^2 p_X(\tilde{x}_i) \tag{7.16}$$

- The *standard deviation*

$$\sigma \equiv \sqrt{\mathrm{Var}[X]} \tag{7.17}$$

The expectation value describes the "average" one would typically obtain if the random experiment is repeated very often. The variance is a measure for the spread of the different outcomes of random variable. As example, the Bernoulli distribution exhibits

$$\begin{aligned} \mathrm{E}[X] &= 0p(0) + 1p(1) = p & (7.18)\\ \mathrm{Var}[X] &= (0-p)^2 p(0) + (1-p)^2 p(1) \\ &= p^2(1-p) + (1-p)^2 p = p(1-p) & (7.19) \end{aligned}$$

One can calculate expectation values of functions $g(x)$ of random variables X via $\mathrm{E}[g(X)] = \sum_i g(\tilde{x}_i) p_X(\tilde{x}_i)$. For the calculation here, we only need that the calculation of the expectation value is a linear operation. Hence, for numbers α_1, α_2 and, in general, two random variables X_1, X_2 one has

$$E[\alpha_1 X_1 + \alpha_2 X_2] = \alpha_1 \,\mathrm{E}[X_1] + \alpha_2 \,\mathrm{E}[X_2]\,. \tag{7.20}$$

In this way, realizing that $\mathrm{E}[X]$ is a number, one obtains:

$$\begin{aligned} \sigma^2 = \mathrm{Var}(X) &= \mathrm{E}[(X - \mathrm{E}[X])^2] = \mathrm{E}[X^2] - 2\,\mathrm{E}[X\ \mathrm{E}[X]] + \mathrm{E}[\mathrm{E}[X]^2] \\ &= \mathrm{E}[X^2] - \mathrm{E}[X]^2 = \mathrm{E}[X^2] - \mu^2 & (7.21)\\ \Leftrightarrow \quad \mathrm{E}[X^2] &= \sigma^2 + \mu^2 & (7.22) \end{aligned}$$

The variance is *not linear*, which can be seen when looking at a linear combination of two *independent* random variables X_1, X_2 (implying $\mathrm{E}[X_1 X_2] =$

$\mathrm{E}[X_1]\,\mathrm{E}[X_2]$ $(\star)$)

$$\begin{aligned}
\sigma^2_{\alpha_1 X_1+\alpha_2 X_2} &= \mathrm{Var}[\alpha_1 X_1 + \alpha_2 X_2] \\
&\overset{(7.21)}{=} \mathrm{E}[(\alpha_1 X_2 + \alpha_2 X_2)^2] - \mathrm{E}[\alpha_1 X_1 + \alpha_2 X_2]^2 \\
&\overset{(7.20)}{=} \mathrm{E}[\alpha_1^2 X_1^2 + 2\alpha_1\alpha_2 X_1 X_2 + \alpha_2^2 X_2^2] \\
&\quad -(\alpha_1\,\mathrm{E}[X_1] + \alpha_2\,\mathrm{E}[X_2])^2 \\
&\overset{(7.20),(\star)}{=} \alpha_1^2\,\mathrm{E}[X_1^2] + \alpha_2^2\,\mathrm{E}[X_2^2] - \alpha_1^2\,\mathrm{E}[X_1]^2 + \alpha_2^2\,\mathrm{E}[X_2]^2 \\
&\overset{(7.21)}{=} \alpha_1^2\,\mathrm{Var}[X_1] + \alpha_2^2\,\mathrm{Var}[X_2] \qquad (7.23)
\end{aligned}$$

The expectation values $E[X^n]$ are called the *n'th moments* of the distribution. This means that the expectation value is the first moment and the variance can be calculated from the first and second moments.

Next, we describe two more important distributions of discrete random variables. First, if one repeats a Bernoulli experiment n times, one can measure how often the result "1" was obtained. Formally, this can be written as a sum of n random variables $X^{(i)}$ which are Bernoulli distributed: $X = \sum_{i=1}^{n} X^{(i)}$ with parameter p. This is a very simple example of a transformation of a random variable, see page 6. In particular, the transformation is linear. The probability to obtain x times the result "1" is calculated as follows: The probability to obtain exactly x times a "1" is p^x, the other $n-x$ experiments yield "0" which happens with probability $(1-p)^{n-x}$. Furthermore, there are $\binom{n}{x} = n!/(x!(n-x)!)$ different sequences with x times "1" and $n-x$ times "0". Hence, one obtains:

Definition The *binomial distribution* with parameters $n \in \mathbb{N}$ and p $(0 < p \leq 1)$ describes a random variable X which has the pmf

$$p_X(x) = \binom{n}{x} p^x (1-p)^{n-k} \quad (0 \leq x \leq n) \qquad (7.24)$$

A common notation is $X \sim B(n,p)$.

Note that the probability mass function is assumed to be zero for argument values that are not stated. A sample plot of the distribution for parameters $n = 10$ and $p = 0.4$ is shown in the left of Fig. 7.2. The Binomial distribution has expectation value and variance

$$\mathrm{E}[X] = np \qquad (7.25)$$

$$\mathrm{Var}[X] = np(1-p) \qquad (7.26)$$

(without proof here). The distribution function cannot be calculated analytically in closed form.

In the limit of a large number of experiments ($n \to \infty$), constrained such that the expectation value $\mu = np$ is kept fixed, the pmf of a Binomial distribution is well approximated by the pmf of the *Poisson distribution*, which is defined as follows: **Definition** The *Poisson distribution* with parameter $\mu > 0$ describes a random variable X with pmf

$$p_X(x) = \frac{\mu^x}{x!} e^{-\mu} \qquad (7.27)$$

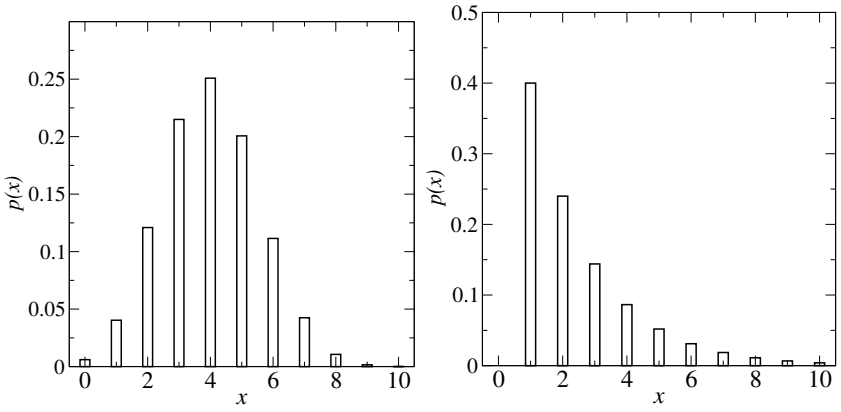


Figure 7.2: (Left) Probability mass function of the binomial distribution for parameters $n = 10$ and $p = 0.4$. (Right) Probability mass function of the geometric distribution for parameter $p = 0.4$.

Indeed, as required, the probabilities sum up to 1, since $\sum_i \frac{\mu^x}{x!}$ is the Taylor series of e^μ. The Poisson distribution exhibits $\mathrm{E}[X] = \mu$ and $\mathrm{Var}[X] = \mu$. Again, a closed form for the distribution function is not known.

Furthermore, one could repeat a Bernoulli experiment just until the first time a "1" is observed, without limit for the number of trials. If a "1" is observed for the first time after exactly x times, then the first $x-1$ times the outcome "0" was observed. This happens with probability $(1-p)^{x-1}$. At the x'th experiment, the outcome "1" is observed which has the probability p. Therefore one obtains

Definition The *geometric distribution* with parameter p $(0 < p \leq 1)$ describes a random variable X which has the pmf

$$p_X(x) = (1-p)^{x-1}p \quad (x \in \mathbb{N}) \tag{7.28}$$

A sample plot of the pmf (up to $x = 10$) is shown in the right of Fig. 7.2. The geometric distribution has (without proof here) the expectation value $E[X] = 1/p$, the variance $\mathrm{Var}[X] = (1-p)/p^2$ and the following distribution function:

$$F_X(x) = \begin{cases} 0 & x < 1 \\ 1-(1-p)^m & m \leq x < m+1 \quad (m \in \mathbb{N}) \end{cases}$$

7.1.2 Continuous random variables

As stated above, random variables are called continuous if they describe random experiments where outcomes from a subset of the real numbers can be obtained. One may describe such random variables also using the distribution function, see Def. 7.1. For continuous random variables, an alternative description is

possible, equivalent to the pmf for discrete random variables: The probability density function states the probability to obtain a certain number per unit:

Definition For a continuous random variable X with a continuous distribution function F_X, the *probability density function* (pdf) $p_X : \mathbb{R} \to [0,1]$ is given by

$$p_X(x) = \frac{dF_X(x)}{dx} \tag{7.29}$$

Consequently, one obtains, using the definition of a derivative and using Eq. (7.11)

$$F_X(x) = \int_{-\infty}^{x} d\tilde{x}\, p_X(\tilde{x}) \tag{7.30}$$

$$P(x_0 < X \leq x_1) = \int_{x_0}^{x_1} d\tilde{x}\, p_X(\tilde{x}) \tag{7.31}$$

Below some examples for important continuous random variables are presented. First, we extend the definitions Def. 7.1.2 of expectation value and variance to the continuous case:

Definition

- The *expectation value* is

$$\mathrm{E}[X] = \int_{-\infty}^{\infty} dx\, x\, p_X(x) \tag{7.32}$$

- The *variance* is

$$\mathrm{Var}[X] = \mathrm{E}[(X - \mathrm{E}[X])^2] = \int_{\infty}^{-\infty} (x - \mathrm{E}[X])^2 p_X(x) \tag{7.33}$$

Expectation value and variance have the same properties as for the discrete case, i.e., Eqs. (7.20), (7.21), and (7.23) hold as well. Also the definition of the n'th moment of a continuous distribution is the same.

Another quantity of interest is the *median*, which describes the central point of the distribution. It is given by the point such that the cumulative probabilities left and right of this point are both equal to 0.5: **Definition** The *median* $x_{\mathrm{med}} = \mathrm{Med}[X]$ is defined via

$$F(x_{\mathrm{med}}) = 0.5 \tag{7.34}$$

The simplest distribution is the uniform distribution, where the probability density function is nonzero and constant in some interval $[a, b)$: **Definition** The *uniform distribution*, with real-valued parameters $a < b$, describes a random variable X which has the pdf

$$p_X(x) = \begin{cases} 0 & x < a \\ \frac{1}{b-a} & x \leq x < b \\ 0 & x \geq 0 \end{cases} \tag{7.35}$$

One writes $X \sim U(a,b)$. The distribution function simply rises linearly from zero, starting at $x = a$, till it reaches 1 at $x = b$, see for example Eq. 7.10 for the case $a = 0$ and $b = L_x$. The uniform distribution exhibits the expectation value $\mathrm{E}[X] = (a+b)/2$ and variance $\mathrm{Var}[X] = (b-a)^2/12$. Note that via the linear transformation $g(X) = (b-a) * X + a$ one obtains $g(X) \sim U(a,b)$ if $X \sim U(0,1)$. The uniform distribution serves as a basis for the generation of (pseudo) random numbers in a computer, see Sec. 7.2.1. All distributions can be in some way obtained via transformations from one or several uniform distributions, see Secs. 7.2.2–7.2.5.

Probably the most important continuous distribution in the context of simulations is the Gaussian distribution:

Definition The *Gaussian distribution*, also called *normal distribution*, with real-valued parameters μ and $\sigma > 0$, describes a random variable X which has the pdf

$$p_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \tag{7.36}$$

One writes $X \sim N(\mu, \sigma^2)$. The Gaussian distribution has expectation value $\mathrm{E}[X] = \mu$ and variance $\mathrm{Var}[X] = \sigma^2$. A sample plot of the distribution for parameters $\mu = 5$ and $\sigma = 3$ is shown in the left of Fig. 7.3. The Gaussian distribution for $\mu = 0$ and $\sigma = 1$ is called *standard normal distribution* $N(0,1)$. One can obtain any Gaussian distribution from $X_0 \sim N(0,1)$ by applying the transformation $g(X_0) = \sigma X_0 + \mu$. Note that the distribution function for the Gaussian distribution cannot be calculated analytically. Thus, one uses usually numerical integration or tabulated values of $N(0,1)$

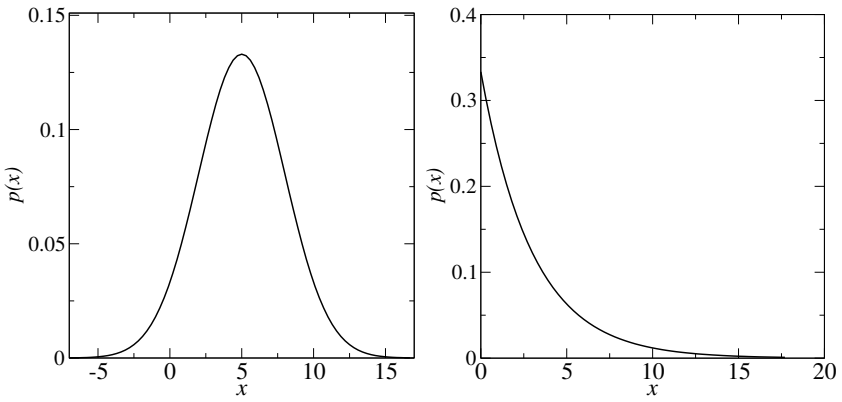


Figure 7.3: (Left) Probability density function of the Gaussian distribution for parameters $\mu = 5$ and $\sigma = 3$. (Right) Probability density function of the exponential distribution for parameter $\mu = 3$.

The *central limit theorem* describes how the Gaussian distribution arises from a sum of random variables:

Theorem Let $X^{(1)}, X^{(2)}, \ldots, X^{(n)}$ be independent random variables, which follow all the same distribution exhibiting expectation value μ and variance σ^2. Then

$$X = \sum_{i=1}^{n} X^{(i)} \tag{7.37}$$

is in the limit of large n approximately Gaussian distributed with mean $n\mu$ and variance $n\sigma^2$, i.e. $X \sim N(n\mu, n\sigma^2)$.

Equivalently, the suitably normalized sum

$$Z = \frac{\frac{1}{n}\sum_{i=1}^{n} X^{(i)} - \mu}{\sigma/\sqrt{n}} \tag{7.38}$$

is approximately standard normal distributed $Z \sim N(0,1)$. For a proof, please refer to standard text books on probability. Since sums of random processes arise very often in nature, the Gaussian distribution is ubiquitous. For instance, the movement of a "large" particle swimming in a liquid called *Brownian motion* is described by a Gaussian distribution.

Another common probability distribution is the exponential distribution. **Definition** The *exponential distribution*, with real-valued parameter $\mu > 0$, describes a random variable X which has the pdf

$$p_X(x) = \frac{1}{\mu} \exp\left(-x/\mu\right) \tag{7.39}$$

A sample plot of the distribution for parameter $\mu = 3$ is shown in the right of Fig. 7.3. The exponential distribution has expectation value $\mathrm{E}[X] = \mu$ and variance $\mathrm{Var}[X] = \mu^2$. The distribution function can be obtained analytically and is given by

$$F_X(x) = 1 - \exp\left(-x/\mu\right) \tag{7.40}$$

The exponential distribution arises under circumstances where processes happen with certain *rates*, i.e., with a constant probability per time unit. Very often, waiting queues or the decay of radioactive atoms are modeled by such random variables. Then the time duration till the first event (or between two events if the experiment is repeated several times) follows Eq. (7.39).

Next, we discuss a distribution, which has attracted recently [Newman (2003), Newman et al. (2006)] much attention in various disciplines like sociology, physics and computer science. Its probability distribution is a power law:

Definition The *power-law distribution*, also called *Pareto distribution*, with real-valued parameters $\gamma > 0$ and $\kappa > 0$, describes a random variable X which has the pdf

$$p_X(x) = \begin{cases} 0 & x < 1 \\ \frac{\gamma}{\kappa}(x/\kappa)^{-\gamma+1} & x \geq 1 \end{cases} \tag{7.41}$$

A sample power-law distribution is shown in Fig. 7.4. When plotting a power-law distribution with double-logarithmic scale, one sees just a straight line.

A discretized version of the power-law distribution appears for example in empirical social networks. The probability that a person has x "close friends" follows a power-law distribution. The same is observed for computer networks for the probability that a computer is connected to x other computers. The power-law distribution has a finite expectation value only if $\gamma > 1$, i.e. if it falls off quickly enough. In that case one obtains $\mathrm{E}[X] = \gamma\kappa/(\gamma - 1)$. Similarly, it exhibits a finite variance only for $\gamma > 2$: $\mathrm{Var}[X] = \frac{\kappa^2\gamma}{(\gamma-1)^2(\gamma-2)}$. The distribution function can be calculated analytically:

$$F_X(x) = 1 - (x/\kappa)^{-\gamma} \quad (x \geq 1) \tag{7.42}$$

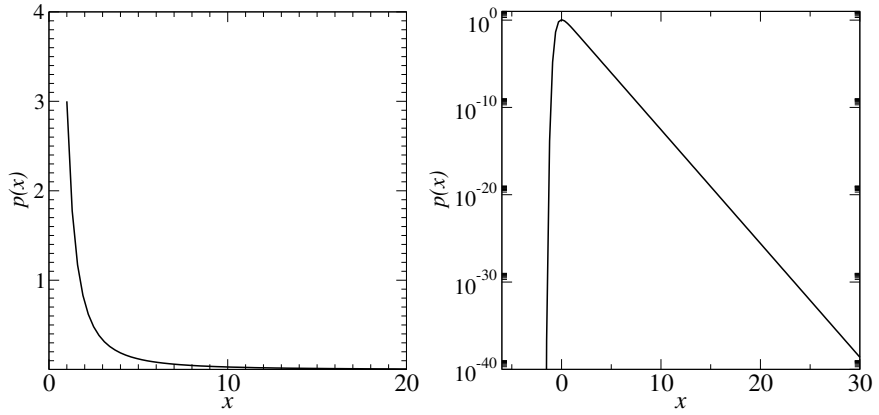


Figure 7.4: (Left) Probability density function of the power-law distribution for parameters $\gamma = 3$ and $\kappa = 1$. (Right) Probability density function of the Fisher-Tippett distribution for parameter $\lambda = 3$ with logarithmically scaled y-axis.

In the context of extreme-value statistics, the Fisher-Tippett distribution (also called log-Weibull distribution) plays an important role.

Definition The *Fisher-Tippett distribution*, with real-valued parameters $\lambda > 0, x_0$, describes a random variable X which has the pdf

$$p_X(x) = \lambda e^{-\lambda x} e^{-e^{-\lambda x}} \tag{7.43}$$

In the special case of $\lambda = 1$, the Fisher-Tippett distribution is also called *Gumbel* distribution. A sample Fisher-Tippett distribution is shown in the right part of Fig. 7.4. The function exhibits a maximum at $x = 0$. This can be shifted to any value μ by replacing x by $x-\mu$. The expectation value is $\mathrm{E}[X] = \nu/\lambda$, where $\nu \equiv 0.57721\ldots$ is the *Euler-Mascheroni constant*. The distribution exhibits a variance of $\mathrm{Var}[X] = \frac{\pi}{\sqrt{6}\lambda}$. Also, the distribution function is known analytically:

$$F_X(x) = e^{-e^{-\lambda x}} \tag{7.44}$$

Mathematically, one can obtain a Gumbel ($\lambda = 1$) distributed random variable from n standard normal $N(0,1)$ distributed variables $X^{(i)}$ by taking the maximum of them and performing the limit $n \to \infty$, i.e. $X = \lim_{n\to\infty} \max\left\{X^{(1)}, X^{(2)}, \ldots, X^{(n)}\right\}$. This is also true for some other "well-behaved" random variables like exponential distributed ones, if they are normalized such that they have zero mean and variance one. The Fisher-Tippett distribution can be obtained from the Gumbel distribution via a linear transformation.

For the estimation of confidence intervals (see Secs. 7.3.2 and 7.3.3) one needs the chi-squared distribution and the F distribution, which are presented next for completeness.

Definition The *chi-squared distribution*, with $\nu > 0$ *degrees of freedom* describes a random variable X which has the probability density function (using the *Gamma function* $\Gamma(x) = \int_0^\infty t^{x-1}e^{-t}\,dt$)

$$p_X(x) = \frac{1}{2^{\nu/2}\Gamma(\nu/2)} x^{\frac{\nu-2}{2}} e^{-\frac{x}{2}} \quad (x > 0) \tag{7.45}$$

and $p_X(x) = 0$ for $x \leq 0$. Distribution function, mean and variance are not stated here. A chi-squared distributed random variable can be obtained from a sum of ν squared standard normal distributed random variables X_i: $X = \sum_{i=1}^{\nu} X_i^2$. The chi-squared distribution is implemented in the *GNU scientific library* (see Sec. 6.3).

Definition The *F distribution*, with $d_1, d_2 > 0$ *degrees of freedom* describes a random variable X which has the pdf

$$p_X(x) = d_1^{d_1/2} d_2^{d_2/2} \frac{\Gamma(d_1/2 + d_2/2)}{\Gamma(d_1/2)\Gamma(d_2/2)} \frac{x^{d_1/2-1}}{(d_1 x + d_2)^{d_1/2+d_2/2}} \quad (x > 0) \tag{7.46}$$

and $p_X(x) = 0$ for $x \leq 0$. Distribution function, mean and variance are not stated here. An F distributed random variable can be obtained from a chi-squared distributed random variable Y_1 with d_1 degrees of freedom and a chi-squared distributed random variable Y_2 with d_2 degrees of freedom via $X = \frac{Y_1/d_1}{Y_2/d_2}$. The F distribution is implemented in the *GNU scientific library* (see Sec. 6.3).

Finally, note that also discrete random variables can be described using probability density functions if one applies the so-called *delta function* $\delta(x - x_0)$. For the purpose of computer simulations this is not necessary. Consequently, no further details are presented here.

7.2 Generating (pseudo) random numbers

For many simulations in science, economy or social sciences, random numbers are necessary. Quite often the model itself exhibits random parameters which remain fixed throughout the simulation; one speaks of *quenched disorder*. A famous example in the field of condensed matter physics are *spin glasses*, which

are random alloys of magetic and non-magnetic materials. In this case, when one performs simulations of small systems, one has to perform an average over different disorder realizations to obtain physical quantities. Each realization of the disorder consists of randomly chosen positions of the magnetic and non-magnetic particles. To generate a disorder realization within the simulations, random numbers are required.

But even when the simulated system is not inherently random, very often random numbers are required by the algorithms, e.g., to realize a finite-temperature ensemble or when using randomized algorithms. In summary, the application of random numbers in computer simulations is ubiquitous.

In this section an introduction to the generation of random numbers is given. First it is explained how they can be generated at all on a computer. Then, different methods are presented for obtaining numbers which obey a target distribution: the *inversion method*, the *rejection method* and *Box-Müller method*. More comprehensive information about these and similar techniques can be found in Refs. [Morgan (1984), Devroye (1986), Press et al. (1995)]. In this section it is assumed that you are familiar with the basic concepts of probability theory and statistics, as presented in Sec. 7.1.

7.2.1 Uniform (pseudo) random numbers

First, it should be pointed out that standard computers are deterministic machines. Thus, it is completely impossible to generate true random numbers directly. One could, for example, include interaction with the user. It is, for example, possible to measure the time interval between successive keystrokes, which is randomly distributed by nature. But the resulting time intervals depend heavily on the current user which means the statistical properties cannot be controlled. On the other hand, there are external devices, which have a true random physical process built in and which can be attached to a computer [Qantis, Westphal] or used via the internet [Hotbits]. Nevertheless, since these numbers are really random, they do not allow to perform stochastic simulations in a controlled and reproducible way. This is important in a scientific context, because spectacular or unexpected results are often tried to be reproduced by other research groups. Also, some program bugs turn up only for certain random numbers. Hence, for debugging purposes it is important to be able to run exactly the same simulation again. Furthermore, for the true random numbers, either the speed of random number generation is limited if the true random numbers are cheap, or otherwise the generators are expensive.

This is the reason why *pseudo random numbers* are usually taken. They are generated by deterministic rules. As basis serves a number generator function `rand()` for a uniform distribution. Each time `rand()` is called, a new (pseudo) random number is returned. (Now the "pseudo" is omitted for convenience) These random numbers should "look like" true random numbers and should have many of the properties of them. One says they should be "good". What "look like" and "good" means, has to be specified: One would like to have a random number generator such that each possible number has indeed the

same probability of occurrence. Additionally, if two generated numbers r_i, r_k differ only slightly, the random numbers r_{i+1}, r_{k+1} returned by the respective subsequent calls should differ sustancially, hence consecutive numbers should have a low correlation. There are many ways to specify a correlation, hence there is no unique criterion. Below, the simplest one will be discussed.

The simplest methods to generate pseudo random numbers are *linear congruential generators*. They generate a sequence $x_1, x_2, \ldots$ of integer numbers between 0 and $m-1$ by a recursive rule:

$$x_{n+1} = (ax_n + c) \mathrm{mod}\, m\,. \tag{7.47}$$

The initial value x_0 is called *seed*. Here we show a simple C implementation `lin_con()`. It stores the current number in the local variable `x` which is declared as `static`, such that it is remembered, even when the function is terminated (see Sec. 1.2). There are two arguments. The first argument `set_seed` indicates whether one wants to set a seed. If yes, the new seed should be passed as second argument, otherwise the value of the second argument is ignored. The function returns the seed if it is changed, or the new random number. Note that the constants a and c are defined inside the function, while the modulus M is implemented via a macro `RNG_MODULUS` to make it visible outside `lin_con()`:

GET SOURCE CODE
DIR: `randomness` FILE(S): `rng.c`

```
#define RNG_MODULUS  32768                  /* modulus */

int lin_con(int set_seed, int seed)
{
  static int x = 1000;        /* current random number */
  const int a = 12351;                    /* multiplier */
  const int c = 1;                             /* shift */


  if(set_seed)                             /* new seed ? */
    x = seed;
  else                           /* new random number ? */
    x = (a*x+c) % RNG_MODULUS;

  return(x);
}
```

If you just want to obtain the next random number, you do not care about the seed. Hence, we use for convenience `rn_lin_con()` to call `lin_con()` with the first argument being 0:

```
int rand_lin_con()
{
  return(lin_con(0,0));
}
```

If we want to set the seed, we also use for convenience a special trivial function `seed_lin_con()`:

```
1 void srand_lin_con(int seed)
2 {
3   lin_con(1, seed);
4 }
```

To generate random numbers r distributed in the interval $[0, 1)$ one has to divide the current random number by the modulus m. It is desirable to obtain equally distributed outcomes in the interval, i.e. a uniform distribution. Random numbers generated from this distribution can be used as input to generate random numbers distributed according to other, basically arbitrary, distributions. Below, you will see how random numbers obeying other distributions can be generated. The following simple C function generates random numbers in $[0, 1)$ using the macro `RNG_MODULUS` defined above:

```
1 double drand_lin_con()
2 {
3   return( (double) lin_con(0,0) / RNG_MODULUS);
4 }
```

One has to choose the parameters a, c, m in a way that "good" random numbers are obtained, where "good" means "with less correlations". Note that in the past several results from simulations have been proven to be wrong because of the application of bad random number generators [Ferrenberg et al. (1992), Vattulainen et al. (1994)].

Example To see what "bad generator" means, consider as an example the parameters $a = 12351, c = 1, m = 2^{15}$ and the seed value $I_0 = 1000$. 10000 random numbers are generated by dividing each of them by m. They are distributed in the interval $[0, 1)$. In Fig. 7.5 the distribution of the random numbers is shown.

The distribution looks rather flat, but by taking a closer look some regularities can be observed. These regularities can be studied by recording k-tuples of k successive random numbers $(x_i, x_{i+1}, \ldots, x_{i+k-1})$. A good random number generator, exhibiting no correlations, would fill up the k-dimensional space uniformly. Unfortunately, for linear congruential generators, instead the points lie on $(k-1)$-dimensional planes. It can be shown that there are *at most* of the order $m^{1/k}$ such planes. A bad generator has much fewer planes. This is the case for the example studied above, see top part of Fig. 7.6

The result for $a = 123450$ is even worse: only 15 different "random" numbers are generated (with seed 1000), then the iteration reaches a fixed point (not shown in a figure).

If instead $a = 12349$ is chosen, the two-point correlations look like that shown in the bottom half of Fig. 7.6. Obviously, the behavior is much more irregular, but poor correlations may become visible for higher k-tuples.

A generator which has passed several empirical tests is $a = 7^5 = 16807$, $m = 2^{31} - 1$, $c = 0$. When implementing this generator you have to be careful,

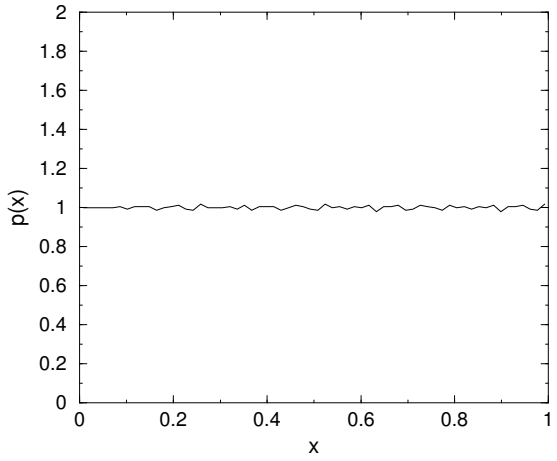


Figure 7.5: Distribution of random numbers in the interval $[0, 1)$ obtained from converting a histogram into a pdf, see Sec. 7.3.3. The random numbers are generated using a linear congruential generator with the parameters $a = 12351, c = 1, m = 2^{15}$.

because during the calculation numbers are generated which do not fit into 32 bit. A clever implementation is presented in Ref. [Press et al. (1995)]. Finally, it should be stressed that this generator, like all linear congruential generators, has the low-order bits much less random than the high-order bits. For that reason, when you want to generate integer numbers in an interval [1,N], you should use

```
r = 1+(int) (N*x_n/m);
```

instead of using the modulo operation as with `r=1+(x_n % N)`.

In standard C, there is a simple built-in random number generator called `rand()` (see corresponding documentation), which has a modulus $m = 2^{15}$, which is very poor. On most operating systems, also `drand48()` is available, which is based on $m = 2^{48}$ ($a =$, $c = 11$) and needs also special arithmetics. It is already sufficient for simulations which no not need many random numbers and do not required highest statistical quality. In recent years, several high-standard random number generators have been developed. Several very good ones are included in the freely availabe *GNU scientific library* (see Sec. 6.3). Hence, you do not have to implement them yourself.

So far, it has been shown how random numbers can be generated which are distributed uniformly in the interval $[0, 1)$. In general, one is interested in obtaining random numbers which are distributed according to a given probability distribution with some density $p(x)$. In the next sections, several techniques suitable for this task are presented.

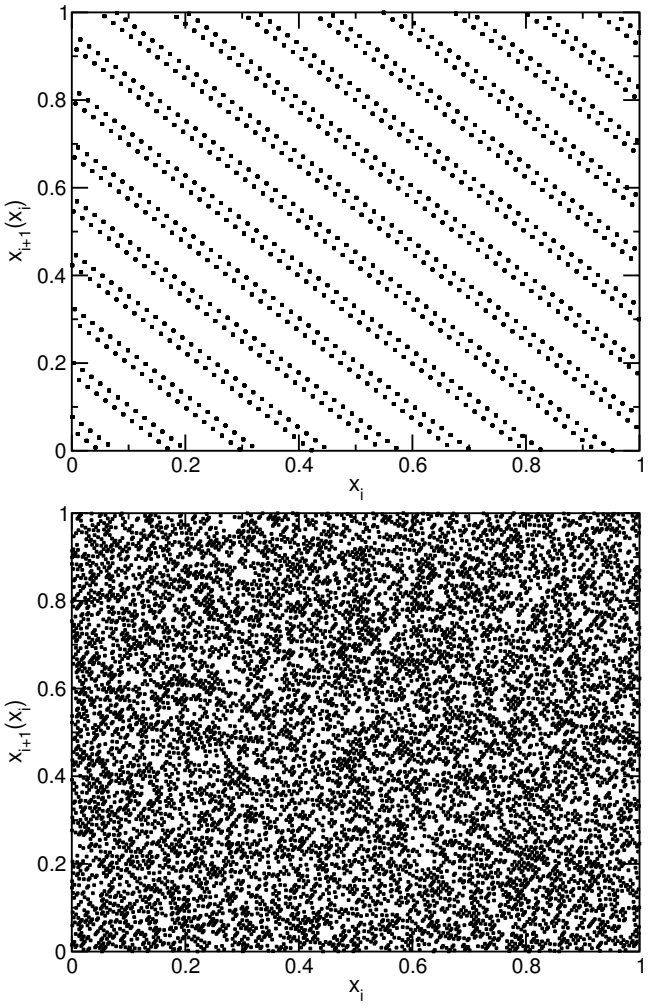


Figure 7.6: Two point correlations $x_{i+1}(x_i)$ between successive random numbers x_i, x_{i+1}. The top case is generated using a linear congruential generator with the parameters $a = 12351, c = 1, m = 2^{15}$, the bottom case has instead $a = 12349$.

7.2.2 Discrete random variables

In case of discrete distributions with finite number of possible outcomes, one can create a table of the possible outcomes together with their probabilities $p_X(x_i)$ $(i = 1, \ldots, i_{\max})$, assuming that the x_i are sorted in ascending order. To draw a number, one has to draw a random number u which is uniformly distributed in $[0, 1)$ and take the entry j of the table such that the sum $s_j \equiv \sum_{i=1}^{j} p_X(x_i)$ of the probabilities is larger than u, but $s_{j-1} \equiv \sum_{i=1}^{j-1} p_X(_i) < u$. Note that one can search the array quickly by *bisection search*: The array is iteratively divided

it into two halves and each time continued in that half where the corresponding entry j is contained. In this way, generating a random number has a time complexity which grows only logarithmically with the number $i_{\max}$ of possible outcomes. This pays off if the number of possible outcomes is very large.

In exercise (1) you are asked to write a function to sample from the probability distribution of a discrete variable, in particular for a Poisson distribution.

In the following, we concentrate on techniques for generating continuous random variables.

7.2.3 Inversion Method

Given is a random number generator `drand()` which is assumed to generate random numbers U which are distributed uniformly in $[0, 1)$. The aim is to generate random numbers Z with probability density $p_Z(z)$. The corresponding distribution function is

$$F_Z(z) \equiv P(Z \leq z) \equiv \int_{-\infty}^{z} dz' p_Z(z') \tag{7.48}$$

The target is to find a function $g(u)$, such that after the transformation $Z = g(U)$ the outcomes of Z are distributed according to (7.48). It is assumed that g can be inverted and is strongly monotonically increasing. Then one obtains

$$F_Z(z) = P(Z \leq z) = P(g(U) \leq z) = P(U \leq g^{-1}(z)) \tag{7.49}$$

Since the distribution function $F_U(u) = P(U \leq u)$ for a uniformly distributed variable is just $F_U(u) = u$ ($u \in [0, 1]$), one obtains $F_Z(z) = g^{-1}(z)$. Thus, one just has to choose $g(z) = F_Z^{-1}(z)$ for the transformation function in order to obtain random numbers, which are distributed according to the probability distribution $F_Z(z)$. Of course, this only works if F_Z can be inverted. If this is not possible, you may use the methods presented in the subsequent sections, or you could generate a table of the distribution function, which is in fact a discretized approximation of the distribution function, and use the methods for generating discrete random numbers as shown in Sec. 7.2.2. This can be even refined by using a linearized approximation of the distribution function. Here, we do not go into further details, but present an example where the distribution function can be indeed inverted.

Example Let us consider the exponential distribution with parameter μ, with distribution function $F_Z(z) = 1 - \exp(-z/\mu)$, see page 14. Therefore, one can obtain exponentially distributed random numbers Z by generating uniform distributed random numbers u and choosing $z = -\mu \ln(1 - u)$.

The following simple C function generates a random number which is exponentially distributed. The parameter μ of the distribution is passed as argument.

GET SOURCE CODE
DIR: `random` FILE(S): `expo.c`

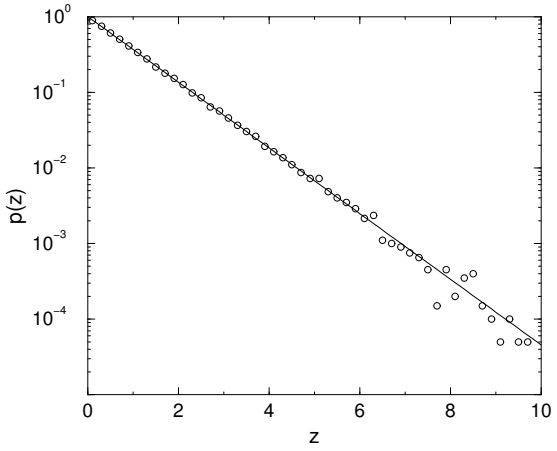


Figure 7.7: Histogram pdf (see page 35) of random numbers generated according to an exponential distribution ($\mu = 1$) compared with the probability density function (straight line) in a logarithmic plot.

```
1 double rand_expo(double mu)
2 {
3   double randnum;                   /* random number U(0,1) */
4   randnum = drand48();
5
6   return(-mu*log(1-randnum));
7 }
```

Note that we use in line 4 the simple `drand48()` random number generator, which is included in the C standard library and works well for applications with moderate statistical requirements. For more sophisticated generates, see e.g. the *GNU scientific library* (see Sec. 6.3).

In Fig. 7.7 a histogram pdf (see page 35) for 10^5 random numbers generated in this way and the exponential probability function for $\mu = 1$ are shown with a logarithmically scaled y-axis. Only for larger values are deviations visible. They are due to statistical fluctuations since $p_Z(z)$ is very small there.

7.2.4 Rejection Method

As mentioned above, the inversion method works only when the distribution function P can be inverted analytically. For distributions not fulfilling this condition, sometimes this problem can be overcome by drawing several random numbers and combining them in a clever way.

The *rejection method* works for random variables where the pdf $p(x)$ fits into a box $[x_0, x_1) \times [0, y_{\max})$, i.e., $p(x) = 0$ for $x \notin [x_0, x_1]$ and $p(x) \leq y_{\max}$. The basic idea of generating a random number distributed according to $p(x)$ is to generate random pairs (x, y), which are distributed uniformly in $[x_0, x_1] \times$

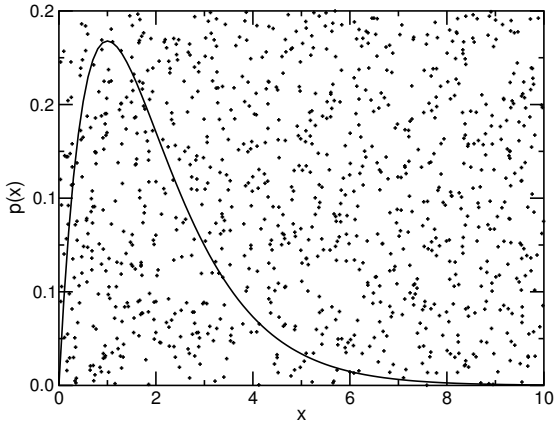


Figure 7.8: The rejection method: Points (x, y) are scattered uniformly over a bounded rectangle. The probability that $y \leq p(x)$ is proportional to $p(x)$.

$[0, y_{\max}]$ and accept only those numbers x where $y \leq p(x)$ holds, i.e., the pairs which are located below $p(x)$, see Fig. 7.8. Therefore, the probability that x is drawn is proportional to $p(x)$, as desired.

The following C function realizes the rejection method for an arbitrary pdf. It takes as arguments the boundaries of the box `y_max`, `x0` and `x1` as well as a pointer `pdf` to the function realizing the pdf. For an explanation of function pointers, see Sec. 1.4.

GET SOURCE CODE
DIR: `randomness` FILE(S): `reject.c`

```
1  double reject(double y_max, double x0, double x1,
2                double (* pdf)(double))
3  {
4    int found;               /* flag if valid number has been found */
5    double x,y;               /* random points in [x0,x1]x[0,p_max] */
6    found = 0;

7    while(!found)                 /* loop until number is generated */
8    {
9      x = x0 + (x1-x0)*drand48();           /* uniformly on [x0,x1] */
10     y = y_max *drand48();               /* uniformly in [0,p_max] */
11     if(y <= pdf(x))                                 /* accept ? */
12       found = 1;
13   }
14   return(x);
15 }
```

In lines 9–10 the random point, which is uniformly distributed in the box, is generated. Lines 11–12 contain the check whether a point below the pdf curve has been found. The search in the loop (lines 7–13) continues until a random number has been accepted, which is returned in line 14.

Example The rejection method is applied to a pdf, which has density 1 in $[0, 0.5)$ and rises linearly from 0 to 4 in $[1, 1.5)$. Everywhere else it is zero. This pdf is realized by the following C function:

```
1  double pdf(double x)
2  {
3    if( (x<0)||
4        ((x>=0.5)&&(x<1))||
5        (x>1.5) )
6        return(0.0);
7    else if((x>=0)&&(x<0.5))
8        return(1.0);
9    else
10       return(4.0*(x-1));
11 }
```

The resulting empirical histogram pdf is shown in Fig. 7.9.

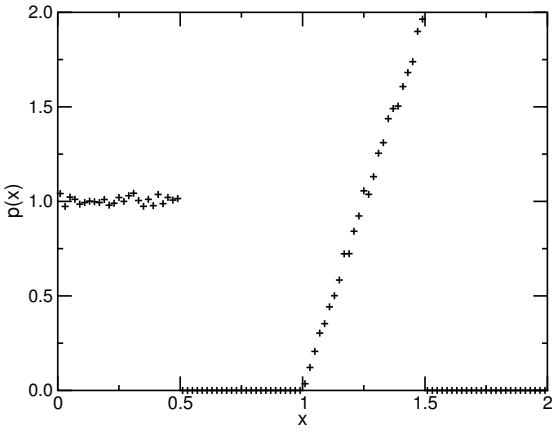


Figure 7.9: Histogram pdf (see page 35) of 10^5 random numbers generated using the rejection method for an artificial pdf.

The rejection method can always be applied if the probability density is boxed, but it has the drawback that more random numbers have to be generated than can be used: If $A = (x_1 - x_0)y_{\max}$ is the area of the box, one has on average to generate $2A$ auxiliary random numbers to obtain one random number of the desired distribution. If this leads to a very poor efficiency, you can consider to use several boxes for different parts of the pdf.

7.2.5 The Gaussian Distribution

In case neither the distribution function can be inverted nor the probability fits into a box, special methods have to be applied. As an example, a method for

generating random numbers distributed according to a Gaussian distribution is considered. Other methods and examples of how different techniques can be combined are collected in [Morgan (1984)].

The probability density function for the Gaussian distribution with mean μ and variance σ^2 is shown in Eq. (7.36), see also Fig. 7.10. It is, apart from uniform distributions, the most common distribution occurring in simulations.

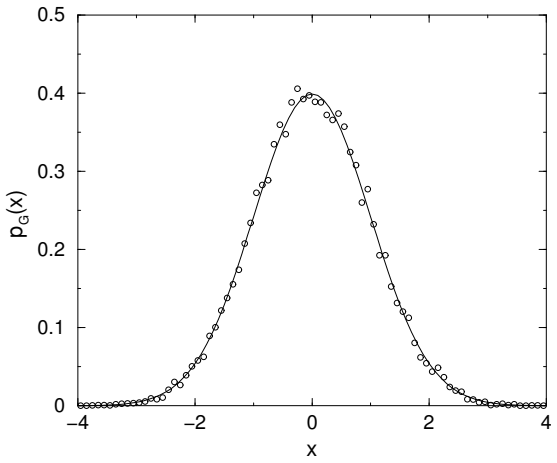


Figure 7.10: Gaussian distribution with zero mean and unit width. The circles represent a histogram pdf (see page 35) obtained from 10^4 numbers drawn with the Box-Müller method.

Here, the case of a standard Gaussian distribution ($\mu = 0,\ \sigma = 1$) is considered. If you want to realize the general case, you have to draw a standard Gaussian distributed number z and then use $\sigma z + \mu$ which is distributed as desired.

Since the Gaussian distribution extends over an infinite interval and because the distribution function cannot be inverted, the methods from above are not applicable. The simplest technique to generate random numbers distributed according to a Gaussian distribution makes use of the central limit theorem 7.1.2. It tells us that any sum of K independently distributed random variables U_i (with mean μ and variance v) will converge to a Gaussian distribution with mean $K\mu$ and variance Kv. If again U_i is taken to be uniformly distributed in $[0, 1)$ (which has mean $\mu = 0.5$ and variance $v = 1/12$), one can choose $K = 12$ and the random variable $Z = \sum_{i=1}^{K} U_i - 6$ will be distributed approximately according to a standard Gaussian distribution. The drawbacks of this method are that 12 random numbers are needed to generate one final random number and that numbers larger than 6 or smaller than -6 will never appear.

In contrast to this technique the *Box-Müller method* is exact. You need two random variables U_1, U_2 uniformly distributed in $[0, 1)$ to generate two independent Gaussian variables N_1, N_2. This can be achieved by generating u_1, u_2 from

U_1, U_2 and assigning

$$\begin{aligned} n_1 &= \sqrt{-2\log(1-u_1)}\cos(2\pi u_2) \\ n_2 &= \sqrt{-2\log(1-u_1)}\sin(2\pi u_2) \end{aligned}$$

A proof that n_1 and n_2 are indeed distributed according to (7.36) can be found e.g. in [Press et al. (1995), Morgan (1984)], where also other methods for generating Gaussian random numbers, some even more efficient, are explained. A method which is based on the simulation of particles in a box is explained in [Fernandez and Criado (1999)]. In Fig. 7.10 a histogram pdf of 10^4 random numbers drawn with the Box-Müller method is shown. Note that you can find an implementation of the Box-Müller method in the solution of Exercise (3).

7.3 Basic data analysis

The starting point is a *sample* of n measured points $\{x_0, x_1, \ldots, x_{n-1}\}$ of some quantity, as obtained from a simulation. Examples are the density of a gas, the transition time between two conformations of a molecule, or the price of a stock. We assume that formally all measurements can be described by random variables X_i representing the same random variable X and that all measurements are statistically independent of each other (treating statistical dependencies is treated in Sec. 7.5). Usually, one does not know the underlying probability distribution $F(x)$, having density $p(x)$, which describes X.

7.3.1 Estimators

Thus, one wants to obtain information about X by looking at the sample $\{x_0, x_1, \ldots, x_{n-1}\}$. In principle, one does this by considering *estimators* $h = h(x_0, x_1, \ldots, x_{n-1})$. Since the measured points are obtained from random variables, $H = h(X_0, X_1, \ldots, X_{n-1})$ is a random variable itself. Estimators are often used to estimate parameters θ of random variables, e.g. moments of distributions. The most fundamental estimators are:

- The *mean*

$$\overline{x} \equiv \frac{1}{n}\sum_{i=0}^{n-1} x_i \tag{7.50}$$

- The *sample variance*

$$s^2 \equiv \frac{1}{n}\sum_{i=0}^{n-1}(x_i - \overline{x})^2 \tag{7.51}$$

  The sample standard deviation is $s \equiv \sqrt{s^2}$.

GET SOURCE CODE
DIR: `randomness` FILE(S): `mean.c`

As example, next a simple C function is shown, which calculates the mean of n data points. The function obtains the number n of data points and an array containing the data as arguments. It returns the average:

```
1  double mean(int n, double *x)
2  {
3    double sum = 0.0;                          /* sum of values */
4    int i;                                          /* counter */
5
6    for(i=0; i<n; i++)          /* loop over all data points */
7      sum += x[i];
8    return(sum/n);
9  }
10
```

You are asked to write a similar function for calculating the variance in exercise (3).

The sample mean can be used to estimate the expectation value $\mu \equiv \mathrm{E}[X]$ of the distribution. This estimate is *unbiased*, which means that the expectation value of the mean, for any sample sizes n, is indeed the expectation value of the random variable. This can be shown quite easily. Note that formally the random variable from which the sample mean $\overline{x}$ is drawn is $\overline{X} = \frac{1}{n}\sum_{i=0}^{n-1} X_i$:

$$\mu_{\overline{X}} \equiv \mathrm{E}[\overline{X}] = \mathrm{E}\left[\frac{1}{n}\sum_{i=0}^{n-1} X_i\right] = \frac{1}{n}\sum_{i=0}^{n-1}\mathrm{E}[X_i] = \frac{1}{n} n\,\mathrm{E}[X] = \mathrm{E}[X] = \mu \qquad (7.52)$$

Here again the linearity of the expectation value was used. The fact that the estimator is unbiased means that if you repeat the estimation of the expectation value via the mean several times, on average the correct value is obtained. This is independent of the sample size. In general, the estimator h for a parameter θ is called unbiased if $\mathrm{E}[h] = \theta$.

Contrary to what you might expect due to the symmetry between Eqs. (7.16) and (7.51), the sample variance is *not* an unbiased estimator for the variance $\sigma^2 \equiv \mathrm{Var}[X]$ of the distribution, but is *biased*. The fundamental reason is, as mentioned above, that $\overline{X}$ is itself a random variable which is described by a distribution $P_{\overline{X}}$. As shown in Eq. (7.52), this distribution has mean μ, independent of the sample size. On the other hand, the distribution has the variance

$$\begin{aligned} \sigma^2_{\overline{X}} &\equiv \mathrm{Var}[\overline{X}] = \mathrm{Var}\left[\frac{1}{n}\sum_{i=0}^{n-1} X_i\right] \overset{(7.23)}{=} \frac{1}{n^2}\sum_{i=0}^{n-1}\mathrm{Var}[X_i] \\ &= \frac{1}{n^2} n\,\mathrm{Var}[X] = \frac{\sigma^2}{n} \end{aligned} \qquad (7.53)$$

Thus, the distribution of $\overline{X}$ gets narrower with increasing sample size n. This has the following consequence for the expectation value of the sample variance which is described by the random variable $S^2 = \frac{1}{n}\sum_{i=0}^{n-1}(X_i - \overline{X})^2$:

$$\begin{aligned}
\mathrm{E}[S^2] &= \mathrm{E}\left[\frac{1}{n}\sum_{i=0}^{n-1}(X_i - \overline{X})^2\right] = \mathrm{E}\left[\frac{1}{n}\sum_{i=0}^{n-1}(X_i^2 - 2X_i\overline{X} + \overline{X}^2)\right] \\
&= \frac{1}{n}\left(\sum_{i=0}^{n-1}\mathrm{E}[X_i^2] - n\,\mathrm{E}[\overline{X}^2]\right) \overset{(7.22)}{=} \frac{1}{n}\left(n(\sigma^2+\mu^2) - n(\sigma_{\overline{X}}^2 + \mu_{\overline{X}}^2)\right) \\
&\overset{(7.53)}{=} \frac{1}{n}\left(n\sigma^2 + n\mu^2 - n\frac{\sigma^2}{n} - n\mu^2\right) = \frac{n-1}{n}\sigma^2 \qquad (7.54)
\end{aligned}$$

This means that, although s^2 is biased, $\frac{n}{n-1}s^2$ is an unbiased estimator for the variance of the underlying distribution of X. Nevertheless, s^2 also becomes unbiased for $n \to \infty$.[1]

For some distributions, for instance a power-law distribution Eq. (7.41) with exponent $\gamma \leq 2$, the variance does not exist. Numerically, when calculating s^2 according Eq. (7.51), one observes that it will not converge to a finite value when increasing the sample size n. Instead one will observe occasionally jumps to higher and higher values. One says the estimator is *not robust*. To get still an impression of the spread of the data points, one can instead calculate the *average deviation*

$$D \equiv \frac{1}{n}\sum_{i=0}^{n-1}|x_i - \overline{x}| \qquad (7.55)$$

In general, an estimator is the less robust, the higher the involved moments are. Even the sample mean may not be robust, for instance for a power-law distribution with $\gamma \leq 1$. In this case one can use the *sample median*, which is the value x_m such that $x_i \leq x_m$ for half the sample points, i.e. x_m is the $(n+1)/2$'th sample point if they are sorted in ascending order.[2] The sample median is clearly an estimator of the median (see Def. 7.1.2). It is more robust, because it is less influenced by the sample points in the tail. The simplest way to calculate the median is to sort all sample points in ascending order and take the sample point at the $(n/2+1)$'th position. This process takes a running time $\mathcal{O}(n \log n)$. Nevertheless, there is an algorithm [Press et al. (1995), Cormen et al. (2001)] which calculates the median even in linear running time $\mathcal{O}(n)$.

7.3.2 Confidence intervals

In the previous section, we have studied estimators for parameters of a random variable X using a sample obtained from a series of independent random

[1] Sometimes the sample variance is defined as $S^\star = \frac{1}{n-1}\sum_{i=0}^{n-1}(x_i - \overline{x})^2$ to make it an unbiased estimator of the variance.

[2] If n is even, one can take the average between the $n/2$'th and the $(n+1)/2$'th sample point in ascending order.

experiments. This is a so-called *point estimator*, because just one number is estimated.

Since each estimator is itself a random variable, each estimated value will be usually off the true value θ. Consequently, one wants to obtain an impression of how far off the estimate might be from the real value θ. This can be obtained for instance from:

Definition The *mean squared error* of a point estimator $H = h(X_0, X_1, \ldots, X_{n-1})$ for a parameter θ is

$$\begin{aligned} \mathrm{MSE}(H) &\equiv \mathrm{E}[(H-\theta)^2] = \mathrm{E}[(H-\mathrm{E}[H]+\mathrm{E}[H]-\theta)^2] \\ &= \mathrm{E}[(H-\mathrm{E}[H])^2] + \mathrm{E}[2(H-\mathrm{E}[H])(\mathrm{E}[H]-\theta)] + \mathrm{E}[(\mathrm{E}[H]-\theta)^2] \\ &= \mathrm{E}[(H-\mathrm{E}[H])^2] + 2\underbrace{(\mathrm{E}[H]-\mathrm{E}[H])}_{=0}(\mathrm{E}[H]-\theta) + (\mathrm{E}[H]-\theta)^2 \\ &= \mathrm{Var}[H] + (\mathrm{E}[H]-\theta)^2 \end{aligned} \tag{7.56}$$

If an estimator is unbiased, i.e., if $\mathrm{E}[H] = \theta$, the mean squared error is given by the variance of the estimator. Hence, if for independent samples (each consisting of n sample points) the estimated values are close to each other, the estimate is quite accurate. Unfortunately, usually only *one* sample is available (how to circumvent this problem rather ingeniously, see Sec. 7.3.4). Also the mean squared error does not immediately provide a probabilistic interpretation of how far the estimate is away from the true value θ.

Nevertheless, one can obtain an estimate of the error in a probabilistic sense. Here we want to calculate a so-called *confidence interval* also sometimes named *error bar*.

Definition For a parameter θ describing a random variable, two estimators $l_\alpha = l_\alpha(x_0, x_1, \ldots, x_{n-1})$ and $u = u_\alpha(x_0, x_1, \ldots, x_{n-1})$ which are obtained from a sample $\{x_0, x_1, \ldots, x_{n-1}\}$ provide a *confidence interval* if, for given *confidence level* $1-\alpha \in (0,1)$ we have

$$P(l_\alpha < \theta < u_\alpha) = 1-\alpha \tag{7.57}$$

The value $\alpha \in (0,1)$ is called conversely *significance level*. This means, the true but unknown value θ is contained in the interval (l, u), which is itself a random variable as well, with probability $1-\alpha$. Typical values of the confidence level are 0.68, 0.95 and 0.99 ($\alpha = 0.32$, 0.05, 0.01, respectively), providing increasing confidence. The more one wants to be sure that the interval really contains the true parameter, i.e. the smaller the value of α, the larger the confidence interval will be.

Next, it is quickly outlined how one arrives at the confidence interval for the mean, for details please consult the specialized literature. First we recall that according to its definition the mean is a sum of independent random variables. For computer simulations, one can assume that usually (see below for a counterexample) a sufficiently large number of experiments is performed.[3] Therefore,

[3] This is different for many empirical experiments, for example, when testing new treat-

according to the central limit theorem 7.1.2 $\overline{X}$ should exhibit (approximately) a pdf $f_{\overline{X}}$ which is Gaussian with an expectation value μ and some variance $\sigma^2_{\overline{X}} = \sigma^2/n$. This means, the probability α that the sample means fall *outside* an interval $I = [\mu - z\sigma_{\overline{X}}, \mu + z\sigma_{\overline{X}}]$ can be easily obtained from the standard normal distribution. This situation is shown in the Fig. 7.11. Note that the interval is symmetric about the mean μ and that its width is stated in multiples $z = z(\alpha)$ of the standard deviation $\sigma_{\overline{X}}$. The relation between significance level α and half interval width z is just $\int_{-z}^{z} dx\, f_{\overline{X}}(x) = 1 - \alpha$. Hence, the weight of the standard normal distribution *outside* the interval $[-z, z]$ is α. This relation can be obtained from any table of the standard Gaussian distribution or from the function `gsl_cdf_gaussian_P()` of the *GNU scientific library* (see Sec. 6.3). Usually, one considers integer values $z = 1, 2, 3$ which correspond to significance levels $\alpha = 0.32$, 0.05, and 0.003, respectively. So far, the confidence interval I

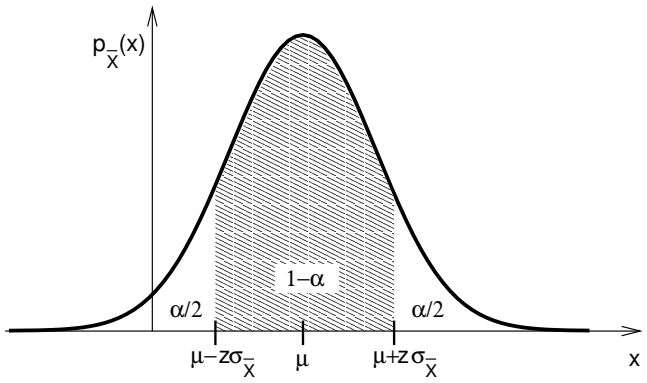


Figure 7.11: Probability density function of the sample mean $\overline{X}$ for large enough sample sizes n where the distribution becomes Gaussian. The true expectation value is denoted by μ and $\sigma_{\overline{X}}$ is the variance of the sample mean. The probability that a random number drawn from this distribution falls outside the symmetric interval $[\mu - z\sigma_{\overline{X}}, \mu + z\sigma_{\overline{X}}]$ is α.

contains the unknown expectation value μ and the unknown variance $\sigma_{\overline{X}}$. First, one can rewrite

$$\begin{aligned} 1 - \alpha &= P(\mu - z\sigma_{\overline{X}} \leq \overline{X} \leq \mu + z\sigma_{\overline{X}}) \\ &= P(-z\sigma_{\overline{X}} \leq \overline{X} - \mu \leq z\sigma_{\overline{X}}) \\ &= P(-\overline{X} - z\sigma_{\overline{X}} \leq -\mu \leq -\overline{X}z\sigma_{\overline{X}}) \\ &= P(\overline{X} - z\sigma_{\overline{X}} \leq \mu \leq \overline{X} + z\sigma_{\overline{X}})\,. \end{aligned}$$

This now states the probability that the true value, which is estimated by the sample mean $\overline{x}$, lies within an interval which is symmetric about the estimate $\overline{x}$.

ments in medical sciences, where often only a very restricted number of experiments can be performed. In this case, one has to consider special distributions, like the *Student distribution*.

Note that the width $2z\sigma_{\overline{X}}$ is basically given by $\sigma_{\overline{X}} = \sqrt{\mathrm{Var}[\overline{X}]}$. This explains why the mean squared error $\mathrm{MSE}(H) = \mathrm{Var}[H]$, as presented in the beginning of this section, is a good measure for the statistical error made by the estimator. This will be used in Sec. 7.3.4.

To finish, we estimate the true variance σ^2 using $\frac{n}{n-1}s^2$, hence we get $\sigma_{\overline{X}} = \frac{\sigma}{\sqrt{n}} \approx \frac{S}{\sqrt{n-1}}$. To summarize we get:

$$P\left(\overline{X} - z\frac{S}{\sqrt{n-1}} \le \mu \le \overline{X} + z\frac{S}{\sqrt{n-1}}\right) \approx 1 - \alpha \qquad (7.58)$$

Note that this confidence interval, with $l_\alpha = \overline{x} - z(\alpha)S/\sqrt{n-1}$ and $u_\alpha = \overline{x} + z(\alpha)S/\sqrt{n-1}$, is symmetric about $\overline{x}$, which is not necessarily the case for other confidence intervals. Very often in scientific publications, to state the estimate for μ including the confidence interval, one gives the range where the true mean is located in 68% of all cases ($z = 1$) i.e. $\overline{x} \pm \frac{S}{\sqrt{n-1}}$, this is called the *standard Gaussian error bar* or *one σ error bar*. Thus, the sample variance and the sample size determine the error bar/ confidence interval.

For the variance, the situation is more complicated, because it is not simply a sum of statistically independent sample points $\{x_0, x_1, \ldots, x_{n-1}\}$. Without going into the details, here only the result from the corresponding statistics literature [Dekking et al (2005), Lefebvre (2006)] is cited: The confidence interval where with probability $1 - \alpha$ the true variance is located is given by $[\sigma_l^2, \sigma_u^2]$ where

$$\begin{aligned} \sigma_l^2 &= \frac{ns^2}{\chi^2(1-\alpha/2, n-1)} \\ \sigma_u^2 &= \frac{ns^2}{\chi^2(\alpha/2, n-1)}\,. \end{aligned} \qquad (7.59)$$

Here, $\chi^2(\beta, \nu)$ is the inverse of the cumulative chi-squared distribution with ν degrees of freedom. It states the value where $F(\chi^2, \nu) = \beta$, see page 16. This chi-squared function is implemented in the *GNU scientific library* (see Sec. 6.3) in the function `gsl_cdf_chisq_Pinv()`.

Note that as one alternative, you could regard $y_i \equiv (x_i - \overline{x})$ approximately as independent data points and use the above standard error estimate described for the mean of the sample $\{y_i\}$. Also, one can use the bootstrap method as explained below (Sec. 7.3.4), which allows to calculate confidence intervals for arbitrary estimators.

7.3.3 Histograms

Sometimes, you do not only want to estimate moments of an underlying distribution, but you want to get an impression of the full distribution. In this case you can use *histograms*.

Definition A histogram is given by a set of disjoint intervals

$$B_k = [l_k, u_k)\,, \tag{7.60}$$

which are called *bins* and a counter h_k for each bin. For a given *sample* of n measured points $\{x_0, x_1, \ldots, x_{n-1}\}$, bin h_k contains the number of sample points x_i which are contained in B_k.

Example For the sample

$$\begin{aligned}\{x_i\} &= \{1.2,\ 1.5,\ 1.0,\ 0.7,\ 1.4,\ 2.0,\\ &\quad\ 1.5,\ 1.1,\ 0.9,\ 1.9,\ 1.2,\ 0.8\}\end{aligned}$$

the bins

$$[0, 0.5),\ [0.5, 1.0)\,[1.0, 1.5),\ [1.5, 2.0),\ [2.0, 2.5)\,[2.5, 3.0)\,,$$

are used, resulting in

$$h_1 = 0,\ h_2 = 3,\ h_3 = 5,\ h_4 = 3,\ h_5 = 1,\ h_6 = 0$$

which is depicted in Fig. 7.12.

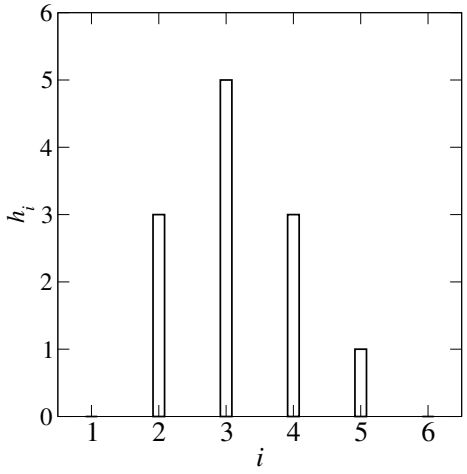


Figure 7.12: Histogram for the data shown in Ex. 7.3.3.

In principle, the bins can be chosen arbitrarily. You should take care that the union of all intervals covers all (possible or actual) sample points. Here, it is

assumed that the bins are properly chosen. Note also that the width $b_k = u_k - l_k$ of each bin can be different. Nevertheless, often bins with uniform width are used. Furthermore, for many applications, for instance, when assigning different weights to different sample points[4], it is useful to consider the counters as real-valued variables. A simple (fixed-bin width) C implementation of histograms is described in Sec. 3.2. The *GNU scientific library* (see Sec. 6.3) contains data structures and functions which implement histograms allowing for variable bin width.

Formally, for a given random variable X, the count h_k in bin k can be seen as a result of a random experiment for the binomial random variable $H_k \sim B(n, p_k)$ with parameters n and p_k, where $p_k = P(X \in B_k)$ is the probability that a random experiment for X results in a value which is contained in bin B_k. This means that confidence intervals for a histogram bin can be obtained in principle from a binomial distribution. Nevertheless, for each sample the true value for a value p_k is unknown and can only be estimated by $q_k \equiv h_k/n$. Hence, the true binomial distribution is unknown. On the other hand, a binomial random variable is a sum of n Bernoulli random variables with parameter p_k. Thus, the estimator q_k is nothing else than a sample mean for a Bernoulli random variable. If the number of sample points n is "large" (see below), from the central limit theorem 7.1.2 and as discussed in Sec. 7.3.2, the distribution of the sample mean (being binomial in fact) is approximately Gaussian. Therefore, one can use the standard confidence interval Eq. (7.58), in this case

$$P\left(q_k - z\frac{S}{\sqrt{n-1}} \le p_k \le q_k + z\frac{S}{\sqrt{n-1}}\right) \approx 1 - \alpha \tag{7.61}$$

Here, according Eq. (7.19), the Bernoulli random variable exhibits a sample variance $s^2 = q_k(1-q_k) = (h_k/n)(1-h_k/n)$. Again, $z = z(\alpha)$ denotes the half width of an interval $[-z, z]$ such that the weight of the standard normal distribution outside the interval equals α. Hence, the estimate with standard error bar ($z = 1$) is $q_k \pm \sqrt{q_k(1-q_k)/(n-1)}$.

The question remains: What is "large" such that you can trust this "Gaussian" confidence interval? Consider that you measure for example no point at all for a certain bin B_k. This can happen easily in the regions where p_k is smaller than $1/n$ but non-zero, i.e. in regions of the histogram which are used to sample the tails of a probability density function. In this case the estimated fraction can easily be $q_k = 0$ resulting also in a zero-width confidence interval, which is certainly wrong. This means, the number of samples n needed to have a reliable confidence interval for a bin B_k depends on the number of bin entries. A rule of thumb from the statistics literature is that $nq_k(1-q_k) > 9$ should hold. If this condition is not fulfilled, the correct confidence interval $[q_{i,l}, q_{i,u}]$ for q_k has to be obtained from the binomial distribution and it is quite complicated, since it uses the *F distribution* (see Def. 7.1.2 on page 16)

[4] This occurs for some advanced simulation techniques.

$$\begin{aligned} q_{i,l} &= \frac{h_k}{h_k + (n - h_k + 1)F_1} \\ q_{i,u} &= \frac{(h_k + 1)F_2}{(h_k + 1)F_2 + n - h_k}\,, \\ \text{where } F_1 &= F(1 - \alpha/2;\, 2n - 2h_k + 2,\, 2h_k) \\ F_2 &= F(1 - \alpha/2;\, 2h_k + 2,\, 2n - 2h_k) \end{aligned} \tag{7.62}$$

The value $F(\beta;\, r_1,\, r_2)$ states the x value such that the distribution function for the F distribution with number of degrees r_1 and r_2 reaches the value β. This inverse distribution function is implemented in the *GNU scientific library* (see Sec. 6.3). If you always use these confidence intervals, which are usually *not* symmetric about q_k, then you cannot go wrong. Nevertheless, for most applications the standard Gaussian error bars are fine.

Finally, in case you want to use a histogram to represent a sample from a continuous random variable, you can easily interpret a histogram as a sample for a probability density function, which can be represented as a set of points $\{(\tilde{x}_k, p(\tilde{x}_k))\}$. This is called the *histogram pdf* or the *sample pdf*. For simplicity, it is assumed that the interval mid points of the intervals are used as x-coordinate. For the normalization, we have to divide by the total number of counts, as for $q_k = h_k/n$ and to divide by the bin width. This ensures that the integral of the sample pdf, approximated by a sum, gives just unity. Therefore, we get

$$\begin{aligned} \tilde{x}_k &\equiv (l_k + u_k)/2 \\ p(\tilde{x}_k) &\equiv h_k/(nb_k)\,. \end{aligned} \tag{7.63}$$

The confidence interval, whatever type you choose, has to be normalized in the same way. A function which prints a histogram as pdf, with simple Gaussian error bars, is shown in Sec. 3.2.

For discrete random variables, the histogram can be used to estimate the pmf.[5]. In this case the choice of the bins, in particular the bin widths, is easy, since usually all possible outcomes of the random experiments are known. For a histogram pdf, which is used to describe approximately a continuous random variable, the choice of the bin width is important. Basically, you have to adjust the width manually, such that the sample data is respresented "best". Thus, the bin width should not be too small nor too large. Sometimes a non-uniform bin width is the best choice. In this case no general advice can be given, except that the bin width should be large where few data points have been sampled. This means that each bin should contain roughly the same number of sample points. Several different rules of thumb exist for uniform bin widths. For example $b = 3.49Sn^{-1/3}$ [Scott (1979)], which comes from minimizing the mean integrated squared difference between a Gaussian pdf and a sample drawn

[5]For discrete random variables, the q_k values are already suitably normalized

from this Gaussian distribution. Hence, the larger the variance S of the sample, the larger the bin width, while increasing the number of sample points enables the bin width to be reduced.

In any case, you should be aware that the histogram pdf can be only an approximation of the real pdf, due to the finite number of data points and due to the underlying discrete nature resulting from the bins. The latter problem has been addressed in recent years by so-called *kernel estimators* [Dekking et al (2005)]. Here, each sample point x_i is represented by a so-called *kernel function*. A kernel function $k(x)$ is a peaked function, formally exhibiting the following properties:

- It has a maximum at 0.
- It falls off to zero over some some distance h.
- Its integral $\int k(x)\,dx$ is normalized to one.

Often used kernel functions are, e.g., a triangle, a cut upside-down parabola or a Gaussian function. Each sample point x_i is represented such that a kernel function is shifted having the maximum at x_i. The estimator $\hat{p}(x)$ for the pdf is the suitably normalized sum (factor $1/n$) of all these kernel functions, one for each sample point:

$$\hat{p}(x) = \frac{1}{n} \sum_i k(x - x_i) \tag{7.64}$$

The advantages of these kernel estimators are that they result usually in a smooth function $\hat{p}$ and that for a value $\hat{p}(x)$ also sample points more distant from x may contribute, with decreasing weight for increasing distance. The most important parameter is the width h, because too small a value of h will result in many distinguishable peaks, one for each sample point, while too large value a of h leads to a loss of important details. This is of similar importance as the choice of the bin width for histograms. The choice of the kernel function (e.g. a triangle, an upside-down parabola or a Gaussian function) seems to be less important.

7.3.4 Resampling using Bootstrap

As pointed out, an estimator for some parameter θ, given by a function $h(x_0, x_1, \ldots, x_{n-1})$, is in fact a random variable $H = h(X_0, X_1, \ldots, X_{n-1})$. Consequently, to get an impression of how much an estimate differs from the true value of the parameter, one needs in principle to know the distribution of the estimator, e.g. via the pdf p_H or the distribution function F_H. In the previous chapter, the distribution was known for few estimators, in particular if the sample size n is large. For instance, the distribution of the sample mean converges to a Gaussian distribution, irrespectively of the distribution function F_X describing the sample points $\{x_i\}$.

For the case of a general estimator H, in particular if F_X is not known, one may not know anything about the distribution of H. In this case one can approximate F_X by the sample distribution function:

Definition For a sample $\{x_0, x_1, \ldots, x_{n-1}\}$, the *sample distribution function* (also called *empirical distribution function*) is

$$F_{\hat{X}}(x) \equiv \frac{\text{number of sample points } x_i \text{ smaller than or equal to } x}{n} \tag{7.65}$$

Note that this distribution function describes in fact a discrete random variable (called $\hat{X}$ here), but is usually (but not always) used to approximate a continuous distribution function.

The *bootstrap principle* is to use $F_{\hat{X}}$ instead of F_X. The name of this principle was made popular by B. Efron [Efron (1979), Efron and Tibshirani (1994)] and comes from the fairy tale of Baron Münchhausen, who dragged himself out of a swamp by pulling on the strap of his boot.[6] Since the distribution function F_X is replaced by the empirical sample distribution function, the approach is also called *empirical bootstrap*, for a variant called parametric bootstrap see below.

Now, having $F_{\hat{X}}$ one could in principle calculate the distribution function $F_{\hat{H}}$ for the random variable $\hat{H} = h(\hat{X}_0, \hat{X}_1, \ldots, \hat{X}_{n-1})$ exactly, which then is an approximation of F_H. Usually, this is to cumbersome and one uses a second approximation: One draws so-called *bootstrap samples* $\{\hat{x}_0, \hat{x}_1, \ldots, \hat{x}_{n-1}\}$ from the random variable $\hat{X}$. This is called *resampling*. This can be done quite simply by n times selecting (*with replacement*) one of the data points of the original sample $\{x_i\}$, each one with the same probability $1/n$. This means that some sample points from $\{x_i\}$ may appear several times in $\{\hat{x}_i\}$, some may not appear at all.[7] Now, one can calculate the estimator value $h^* = h(\hat{x}_0, \hat{x}_1, \ldots, \hat{x}_{n-1})$ for each bootstrap sample. This is repeated K times for different bootstrap samples resulting in K values h^*_k $(k = 1, \ldots, K)$ of the estimator. The sample distribution function F_{H^*} of this sample $\{h^*_k\}$ is the final result, which is an approximation of the desired distribution function F_H. Note that the second approximation, replacing $F_{\hat{H}}$ by F_{H^*} can be made arbitrarily accurate by making K as large as desired, which is computationally cheap.

You may ask: Does this work at all, i.e., is F_{H^*} a good approximation of F_H? For the general case, there is no answer. But for some cases there are mathematical proofs. For example for the mean $H = \overline{X}$ the distribution function $F_{\overline{X}^*}$ in fact converges to $F_{\overline{X}}$. Here, only the subtlety arises that one has to consider in fact the *normalized* distributions of $\overline{X} - \mu$ ($\mu = \mathrm{E}[X]$) and $\hat{X} - \overline{x}$ ($\overline{x} = \sum_{i=0}^{n-1} x_i/n$). Thus, the random variables are just shifted by constant values. For other cases, like for estimating the median or the variance, one has to normalize in a different way, i.e., by subtracting the (empirical) median or by dividing by the (empirical) variance. Nevertheless, for the characteristics of F_H we are interested in, in particular in the variance, see below, normalizations like shifting and stretching are not relevant, hence they are ignored in the following. Note that indeed some estimators exist, like the maximum of a distribution, for which one can prove conversely that F_{H^*} does *not* converge to F_H, even after

[6] In the European version, he dragged himself out by pulling his hair.

[7] The probability for a sample point not to be selected is $(1-1/n)^n = \exp(n \log(1-1/n)) \to \exp(n(-1/n)) = \exp(-1) \approx 0.367$ for $n \to \infty$.

some normalization. On the other hand, for the purpose of getting a not too bad estimate of the error bar, for example, bootstrapping is a very convenient and suitable approach which has received high acceptance during recent years.

Now one can use F_{H*} to calculate any desired quantity. Most important is the case of a confidence interval $[h_l, h_u]$ such that the total probability outside the interval is α, for given significance level α, i.e. $F_{H^*}(h_u) - F_{H^*}(h_l) = 1 - \alpha$. In particular, one can distribute the weight α equally below and above the interval, which allows to determine h_l, h_u

$$F_{H^*}(h_u) = F_{H^*}(h_l) = \alpha/2\,. \tag{7.66}$$

Similar to the confidence intervals presented in Sec. 7.3.2, $[h_l, h_u]$ also represents a confidence interval for the unknown parameter θ which is to be estimated from the estimator (if it is unbiased). Note that $[h_l, h_u]$ can be non-symmetric about the actual estimate $h(x_0, x_1, \ldots, x_{n-1})$. This will happen if the distribution F_{H^*} is skewed.

For simplicity, as we have seen in Sec. 7.3.2, one can use the variance $\mathrm{Var}[H]$ to describe the statistical uncertainty of the estimator. As mentioned on page 32, this corresponds basically to a $\alpha = 0.32$ uncertainty.

GET SOURCE CODE
DIR: `randomness` FILE(S): `bootstrap.c` `bootstrap_test.c`

The following C function calculates $\mathrm{Var}[H^*]$, as approximation of the unknown $\mathrm{Var}[H]$. One has to pass as arguments the number n of sample points, an array containing the sample points, the number K of bootstrap iterations, and a pointer to the function `f` which represents the estimator. `f` has to take two arguments: the number of sample points and an array containing a sample. For an explanation of function pointers, see Sec. 1.4. The function `bootstrap_variance()` returns $\mathrm{Var}[H^*]$.

```
1  double bootstrap_variance(int n, double *x, int n_resample,
2                            double (*f)(int, double *))
3  {
4    double *xb;                                    /* bootstrap sample */
5    double *h;                                /* results from resampling */
6    int sample, i;                                  /* loop counters */
7    int k;                                         /* sample point id */
8    double var;                                /* result to be returned */
9    h = (double *) malloc(n_resample * sizeof(double));
10   xb = (double *) malloc(n * sizeof(double));
11   for(sample=0; sample<n_resample; sample++)
12   {
13     for(i=0; i<n; i++)                                    /* resample */
14     {
15       k = (int) floor(drand48()*n);          /* select random point */
16       xb[i] = x[k];
17     }
18     h[sample] = f(n, xb);                    /* calculate estimator */
19   }
```

```
20    var = variance(n_resample, h);      /* obtain bootstrap variance */
21    free(h);
22    free(xb);
23    return(var);
24  }
```

The bootstrap samples $\{\hat{x}_i\}$ are stored in the array `xb`, while the sampled estimator values $\{h_k^*\}$ are stored in the array `h`. These arrays are allocated in lines 10–11. In the main loop (lines 12–20) the bootstrap samples are calculated, each time the estimator is obtained and the result is stored in `h`. Finally, the variance of the sample $\{h_k^*\}$ is calculated (line 22). Here, the function `variance()` is used, which works similarly to the function `mean()`, see exercise (3). Your are asked to implement a bootstrap function for general confidence interval in exercise (4).

The most obvious way is to call `bootstrap_variance()` with the estimator `mean` as forth argument. For a distribution which is "well behaved" (i.e., where a sum of few random variables resembles the Gaussian distribution), you will get a variance that is, at least if `n_resample` is reasonably large, very close to the standard Gaussian ($\alpha = 0.32$) error bar.

For calculating properties of the sample mean, the bootstrap approach works fine, but in this case one could also be satisfied with the standard Gaussian confidence interval. The bootstrap approach is more interesting for non-standard estimators. One prominent example from the field of statistical physics is the so-called *Binder cumulant* [Binder (1981)], which is given by:

$$b(x_0, x_1, \ldots, x_{n-1}) = 0.5 \left(3 - \frac{\overline{x^4}}{[\overline{x^2}]^2} \right) \tag{7.67}$$

where $\overline{\ldots}$ is again the sample mean, for example $\overline{x^2} = \sum_{i=0}^{n-1} x_i^2$. The Binder cumulant is often used to determine phase transitions via simulations, where only systems consisting of a finite number of particles can be studied. For example, consider a ferromagnetic system held at some temperature T. At low temperature, below the *Curie temperature* T_c, the system will exhibit a macroscopic magnetization m. On the other hand, for temperatures above T_c, m will on average converge to zero when increasing the system size. This transition is fuzzy, if the system sizes are small. Nevertheless, when evaluating the Binder cumulant for different sets of sample points $\{m(T, L)_i\}$ which are obtained at several temperatures T and for different system sizes L, the $b_L(T)$ curves for different L will all cross [Landau and Binder (2000)] (almost) at T_c, which allows for a very precise determination of T_c. A sample result for a two-dimensional (i.e. layered) model ferromagnet exhibiting $L \times L$ particles is shown in Fig. 7.13. The Binder cumulant has been useful for the simulation of many other systems like disordered materials, gases, optimization problems, liquids, and graphs describing social systems.

GET SOURCE CODE

DIR: `randomness`
FILE(S):
`binder_L8.dat`
`binder_L10.dat`
`binder_L16.dat`
`binder_L30.dat`

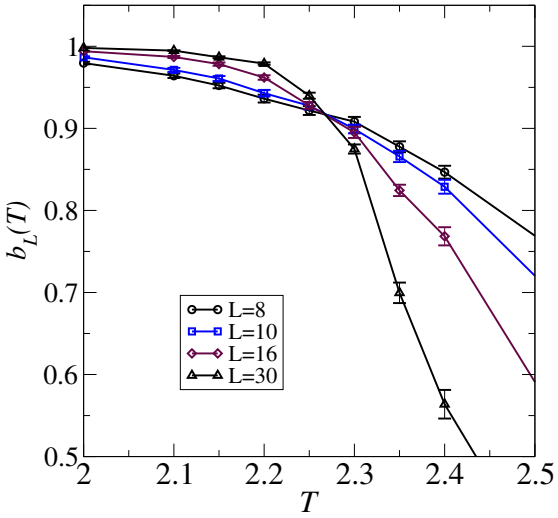


Figure 7.13: Plot of Binder cumulant of two-dimensional model ferromagnet as function of temperature T (dimensionless units). Each system consists of $L \times L$ particles. The curves for different system sizes L cross very close to the phase transition temperature $T_c = 2.269$ (known from analytical calculations of this model). The error bars shown can be obtained using a bootstrap approach.

A confidence interval for the Binder cumulant is very difficult (or even impossible) to obtain using standard error analysis. Using bootstrapping, it is straightforward. You can use simply the function `bootstrap_variance()` shown above while providing as argument a function which evaluates the Binder cumulant for a given set of data points.

So far, it was assumed that the empirical distribution function $F_{\hat{X}}$ was used to determine an approximation of F_H. Alternatively, one can use some additional knwoledge which might be available. Or one can make additional assumptions, via using a distribution function $F_{\underline{\lambda}}$ which is parametrized by a vector of parameters $\underline{\lambda}$. For an exponential distribution, the vector would just consist of one parameter, the expectation value, while for a Gaussian distribution, $\underline{\lambda}$ would consist of the expectation value and the variance. In principle, arbitrary complex distributions with many parameters are possible. To make $F_{\underline{\lambda}}$ a "good" approximation of F_X, one has to adjust the parameters such that the distribution function represents the sample $\{x_i\}$ "best", resulting in a vector $\hat{\underline{\lambda}}$ of parameters. Methods and tools to perform this *fitting* of parameters are presented in Sec. 7.6.2. Using $F_{\hat{\underline{\lambda}}}$ one can proceed as above: Either one calculates $F_{\hat{H}}$ exactly based on $F_{\hat{\underline{\lambda}}}$, which is most of the time too cumbersome. Instead, usually one performs simulations where one takes repeatedly samples $\{\hat{x}_0, \hat{x}_1, \ldots, \hat{x}_{n-1}\}$ from simulating $F_{\hat{\underline{\lambda}}}$ and calculates each time the estimator $h^* = h(\hat{x}_0, \hat{x}_1, \ldots, \hat{x}_{n-1})$. This results, as in the case of the empirical boot-

strap discussed above, in a sample distribution function F_{H^*} which is further analyzed. This approach, where $F_{\underline{\lambda}}$ is used instead of $F_{\hat{X}}$, is called *parametric bootstrap*.

Note that the bootstrap approach does not require that the sample points are statistically independent of each other. For instance, the sample could be generated using a Markov chain Monte Carlo simulation [Newman and Barkema (1999), Landau and Binder (2000), Robert and Casella (2004), Liu (2008)], where each data point x_{i+1} is calculated using some random process, but also depends on the previous data point x_i. More details on how to quantify correlations are given in Sec. 7.5. Nevertheless, if the sample follows the distribution F_X, everything is fine when using bootstrapping and for example a confidence interval will not depend on the fraction of "independent" data points. One can see this easily by assuming that you replace each data point in the original sample $\{x_i\}$ by ten copies, hence making the sample ten times larger without adding any information. This will not affect any of the following bootstrap calculations, since the size of the sample does not enter explicitly. The fact that bootstrapping is not susceptible to correlations between data points is in contrast to the classical calculation of confidence intervals explained in Sec. 7.3.2, where independence of data is assumed and the number of independent data points enters formulas like Eq. (7.58). Hence, when calculating the error bar according to Eq. (7.58) using the ten-copy sample, it will be *incorrectly* smaller by a factor $\sqrt{10}$, since no additional information is available compared to the original sample.

It should be mentioned that bootstrapping is only one of several resampling techniques. Another well known approach is the *jackknife approach*, where one does not sample randomly using $F_{\hat{X}}$ or a fitted $F_{\underline{\lambda}}$. Instead the sample $\{x_i\}$ is divided into B blocks of equal size $n_b = n/B$ (assuming that n is a multiple of B). Note that choosing $B = n$ is possible and not uncommon. Next, a number B of so-called *jackknife samples* $b = 1, \ldots, B$ are formed from the original sample $\{x_i\}$ by omitting exactly the sample points from the b'th block and including all other points of the original sample. Therefore, each of these jackknife samples consists of $n - n_b$ sample points. For each jackknife sample, again the estimator is calculated, resulting in a sample $\{h_k^{(j)}\}$ of size B. Note that the sample distribution function $F^{(j)}$ of this sample is *not* an approximation of the estimator distribution function F_H! Nevertheless, it is useful. For instance, the variance $\mathrm{Var}[H]$ can be estimated from $(B-1)S_h^2$, where S_h^2 is the sample variance of $\{h_k^{(j)}\}$. No proof of this is presented here. It is just noted that when increasing the number B of blocks, i.e., making the different jackknife samples more alike, because fewer points are excluded, the sample of estimators values $\{h_k^{(j)}\}$ will fluctuate less. Consequently, this dependence on the number of blocks is exactly compensated via the factor $(B-1)$. Note that for the jackknife method, in contrast to the boostrap approach, the statistical independence of the original sample is required. If there are correlations between the data points, the jackknife approach can be combined with the so-called blocking method [Flyvbjerg (1998)]. More details on the jackknife approach

can be found in [Efron and Tibshirani (1994)].

Finally, you should be aware that there are cases where resampling approaches clearly fail. The most obvious example is the calculation of confidence intervals for histograms, see Sec. 7.3.3. A bin which exhibits no sample points, for example, where the probability is very small, will never get a sample point during resampling either. Hence, the error bar will be of zero width. This is in contrast to the confidence interval shown in Eq. 7.62, where also bins with zero entries exhibit a finite-size confidence interval. Consequently, you have to think carefully before deciding which approach you will use to determine the reliability of your results.

7.4 Data plotting

So far, you have learned many methods for analyzing data. Since you do not just want to look at tables filled with numbers, you should visualize the data in viewgraphs. Those viewgraphs which contain the essential results of your work can be used in presentations or publications. To analyze and plot data, several commercial and non-commercial programs are available. Here, two free programs are discussed, *gnuplot*, and *xmgrace*. *Gnuplot* is small, fast, allows two- and three-dimensional curves to be generated and transformed, as well as arbitrary functions to be fitted to the data (see Sec. 7.6.2). On the other hand *xmgrace* is more flexible and produces better output. It is recommended to use *gnuplot* for viewing and fitting data online, while *xmgrace* is to be preferred for producing figures to be shown in presentations or publications.

7.4.1 *gnuplot*

The program *gnuplot* is invoked by entering `gnuplot` in a shell, or from a menu of the graphical user interface of your operating system. For a complete manual see [Texinfo].

As always, our examples refer to a UNIX window system like X11, but the program is available for almost all operating systems. After startup, in the window of your shell or the window which pops up for `gnuplot` the prompt (e.g. `gnuplot>`) appears and the user can enter commands in textual form, results are shown in additional windows or are written into files. For a general introduction you can type just `help`.

Before giving an example, it should be pointed out that gnuplot *scripts* can be generated by simply writing the commands into a file, e.g. `command.gp`, and calling `gnuplot command.gp`.

GET SOURCE CODE
DIR: `randomness` FILE(S): `sg_e0_L.dat`

The typical case is that you have available a data file of $x - y$ data or with $x - y - dy$ data (where dy is the error bar of the y data points). Your file might look like this, where the "energy" e_0 of a system[8] is stored as a function of the "system size" L. The filename

[8] It is the ground-state energy of a three-dimensional $\pm J$ spin glass , a protypical system

is `sg_e0_L.dat`. The first column contains the L values, the second the energy values and the third the standard error of the energy. Please note that lines starting with "`#`" are comment lines which are ignored on reading:

```
# ground state energy of +-J spin glasses
# L    e_0   error
  3 -1.6710 0.0037
  4 -1.7341 0.0019
  5 -1.7603 0.0008
  6 -1.7726 0.0009
  8 -1.7809 0.0008
 10 -1.7823 0.0015
 12 -1.7852 0.0004
 14 -1.7866 0.0007
```

To plot the data enter

```
gnuplot> plot "sg_e0_L.dat" with yerrorbars
```

which can be abbreviated as `p "sg_e0_L.dat" w e`. Please do not forget the quotation marks around the file name. Next, a window pops up, showing the result, see Fig. 7.14.

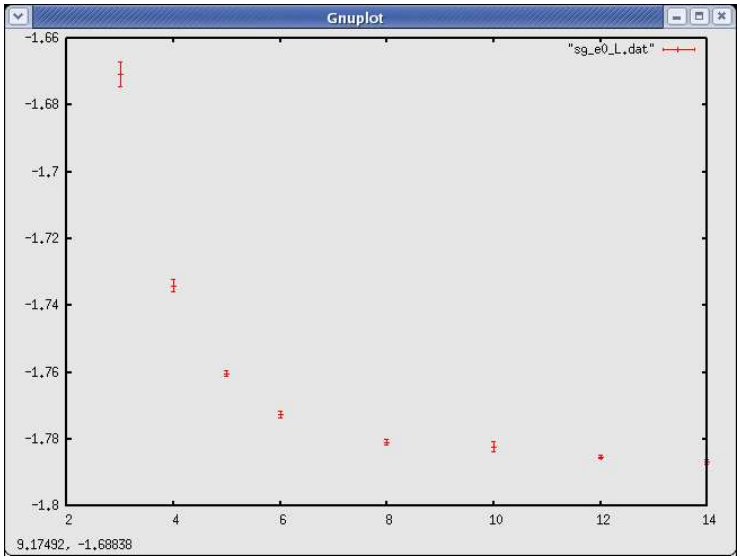


Figure 7.14: *Gnuplot* window showing the result of a plot command.

For the `plot` command many options and styles are available, e.g. `with lines` produces lines instead of symbols. It is not explained here how to set

in statistical physics. These spin glasses model the magnetic behavior of alloys like iron-gold.

line styles or symbol sizes and colors, because this is usually not necessary for a quick look at the data. For "nice" plots used for presentations, we recommend *xmgrace*, see next section. Anyway, `help plot` will tell you all you have to know about the `plot` command.

Among the important options of the `plot` command is that one can specify ranges. This can be done by specifying the range directly after the command, e.g.

```
gnuplot> plot [7:20]  "sg_e0_L.dat" with yerrorbars
```

will only show the data for $x \in [7, 20]$. Also an additional x range can be specified like in

```
plot [7:20][-1.79:-1.77]  "sg_e0_L.dat" with yerrorbars
```

If you just want to set the y range, you have to specify `[ ]` for the x-range. You can also fix the ranges via the `set xrange` and the `set yrange` commands, such that you do not have to give them each time with the plot command, see `help set xrange` or `help unset xrange` for unsetting a range.

`Gnuplot` knows a lot of built-in functions like $\sin(x)$, $\log(x)$, powers, roots, Bessel functions, error function,[9] and many more. For a complete list type `help functions`. These function can be also plotted. Furthermore, using these functions and standard arithmetic expressions, you can also define your own functions, e.g. you can define a function `ft(x)` for the Fischer-Tippett pdf (see Eq. (7.43)) for parameter λ (called `lambda` here) and show the function via

```
gnuplot> ft(x)=lambda*exp(-lambda*x)*exp(-exp(-lambda*x))
gnuplot> lambda=1.0
gnuplot> plot ft(x)
```

You can also include arithmetic expressions in the plot command. To plot a shifted and scaled Fischer-Tippett pdf you can type:

```
gnuplot> plot [0:20] 0.5*ft(0.5*(x-5))
```

The Fischer-Tippett pdf has a tail which drops off exponentially. This can be better seen by a logarithmic scaling of the y axis.

```
gnuplot> set logscale y
gnuplot> plot [0:20] 0.5*ft(0.5*(x-5))
```

will produce the plot shown in Fig. 7.15.

Furthermore, it is also possible to plot several functions in one plot, via separating them via commas, e.g. to compare a Fischer-Tippett pdf to the standard Gaussian pdf, here the predefined constant `pi` is used:

```
gnuplot> plot ft(x), exp(-x*x/2)/sqrt(2*pi)
```

[9] The error function is $\mathrm{erf}(x) = (2/\sqrt{\pi}) \int_0^x dx' \exp(-x'^2)$.

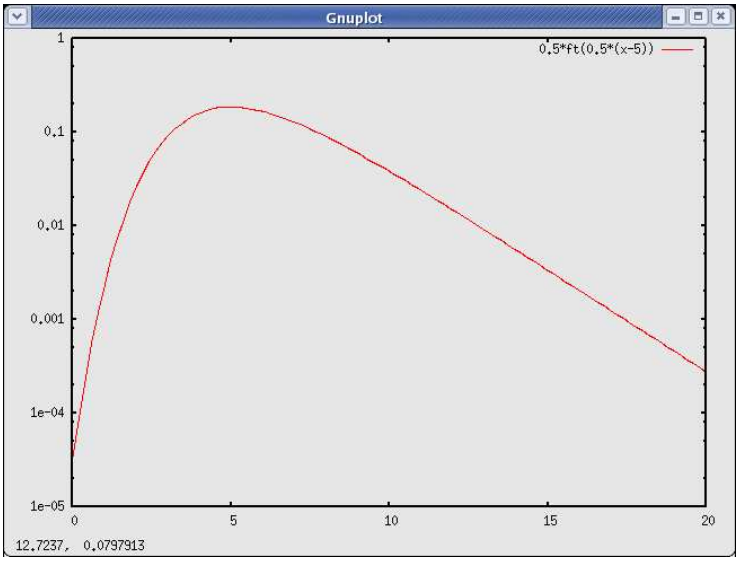


Figure 7.15: *Gnuplot* window showing the result of plotting a shifted and rescaled Fischer-Tippett pdf with logarithmically scaled y-axis.

It is possible to read files with multi columns via the `using` *data modifier*, e.g.

```
gnuplot> plot "test.dat" using 1:4:5 w e
```

displays the fourth column as a function of the first, with error bars given by the 5th column. The elements behind the `using` are called entries. Within the `using` data modifier you can also perform transformations and calculations. Each entry, where some calculations should be performed have to be embraced in `( )` brackets. Inside the brackets you can refer to the different columns of the input file via `$1` for the first column, `$2` for the second, etc. You can generate arbitrary expressions inside the brackets, i.e. use data from different columns (also combine several columns in one entry), operators, variables, predefined and self-defined functions and so on. For example, in Sec. 7.6.2, you will see that the data from the `sg_e0_L.dat` file follows approximately a power law behavior $e_0(L) = e_\infty + aL^b$ with $e_\infty \approx -1.788$, $a \approx 2.54$ and $b \approx -2.8$. To visualize this, we want to show $e_0(L) - e_\infty$ as a function of L^b. This is accomplished via:

```
gnuplot> einf=-1.788
gnuplot> b=-2.8
gnuplot> plot "sg_e0_L.dat" u ($1**b):($2-einf)
```

Now the *gnuplot* window will show the data as a straight line (not shown, but see Fig. 7.23).

So far, all output has appeared on the screen. It is possible to redirect the output, for example, to an encapsulated postscript file (by setting `set terminal postscript` and redirecting the output `set output "test.eps"`). When you now enter a plot command, the corresponding postscript file will be generated.

Note that not only several functions but also several data files or a mixture of both can be combined into one figure. To remember what a plot exported to files means, you can set axis labels of the figure by typing e.g. `set xlabel "L"`, which becomes active when the next `plot` command is executed. Also you can use `set title` or place arbitrary labels via `set label`. Use the `help` command to find out more.

Also three-dimensional plotting (in fact a projection into two dimensions) is possible using the `splot` command (enter `help splot` to obtain more information). Here, as example, we plot a two-dimensional Gaussian distribution:

```
gnuplot> x0=3.0
gnuplot> y0=-1.0
gnuplot> sx=1.0
gnuplot> sy=5.0
gnuplot> gauss2d(x,y)=exp(-(x-x0)**2/(2*sx)-(y-y0)**2/(2*sy))\
> /sqrt(4*pi**2*sx**2*sy**2)
gnuplot> set xlabel "x"
gnuplot> set ylabel "y"
gnuplot> splot [x0-2:x0+2][y0-4:y0+4]  gauss2d(x,y) with points
gnuplot>
```

Note that the long line containing the definition of the (two-argument) function `gauss2d()` is split up into two lines using a backslash at the end of the first line. Furthermore, some of the variables are used inside the interval specifications at the beginning of the `splot` command. Clearly, you also can plot data files with three-dimensional data. The resulting plot appearing in the output window is shown in Fig. 7.16. You can drag the mouse inside the window showing the plot, which will alter the view.

Finally, to stop the execution of *gnuplot*, enter the command `exit`. These examples should give you already a good impression of what can be done with *gnuplot*. More can be found in the documentation or the online help. How to fit functions to data using *gnuplot* is explained in Sec. 7.6.2. It is also possible to make, with some effort, publication-suitable plots, but it is simpler to achieve this with *xmgrace*, which is presented in the following section.

7.4.2 *xmgrace*

The *xmgrace* (X Motiv GRaphing, Advanced Computation and Exploration of data) program is much more powerful than *gnuplot* and produces nicer output, commands are issued by clicking on menus and buttons and it offers WYSIWYG. The *xmgrace* program offers almost every feature you can imagine for two-dimensional data plots, including multiple plots (insets), fits, fast Fourier transform, interpolation. The look of the plots may be altered in any kind of

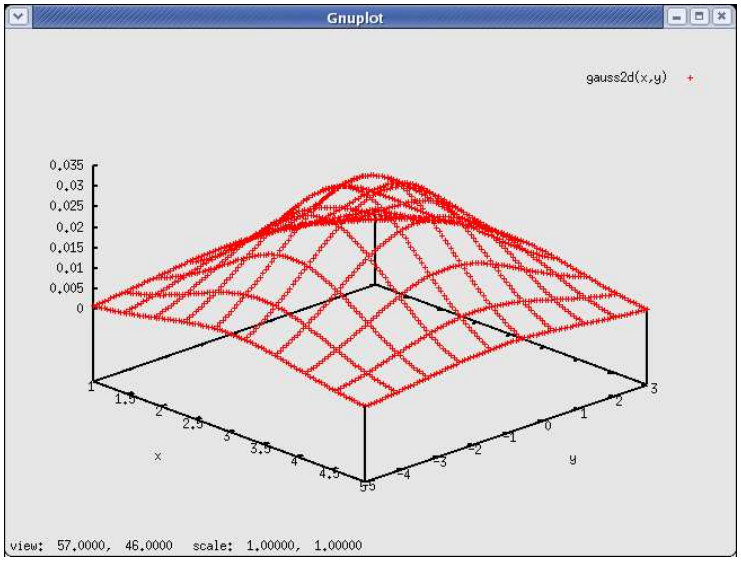


Figure 7.16: *Gnuplot* window showing the result of plotting a two-dimensional function using `splot`.

way you can imagine like choosing fonts, sizes, colors, symbols, styles for lines, bar charts etc. Also, you can create manifold types of labels / legends and it is possible to add elements like texts, labels, lines or other geometrical objects in the plot. The plots can be exported to various format, in particular encapsulated postscript (`.eps`) Advanced users also can program it or use it for real-time visualization of simulations. On the other hand, its handling is a little bit slower compared to *gnuplot* and the program has the tendency to fill your screen with windows. For full information, please consult the online help, the manual or the program's web page [xmgrace].

Here, just the main steps to produce a simple but nice plot are shown and some further directions are mentioned. You will be given here the most important steps to create a similar plot to the first example, shown for the *gnuplot* program, but ready for publication. First you have to start the program by typing `xmgrace` into a shell (or to start it from some window/operating system menu). Then you choose the Data menu[10], next the Import sub menu and finally the ASCII.. sub sub menu. Then a "Grace:Read Set" window will pop up (see Fig. 7.17) and you can choose the data file to be loaded (here `sg_e0_L.dat`) [A], the type of the input file (Single Set) [B], the format of the data (XYDY) [C]. This means you have three columns, and the third one is an error bar for the second. Then you can hit on the OK button [E]. The data will be loaded and

[10]The underlined character appears also in the menu name and refers to the key one has to hit together with Alt button, if one wants to open the menu via key strokes.

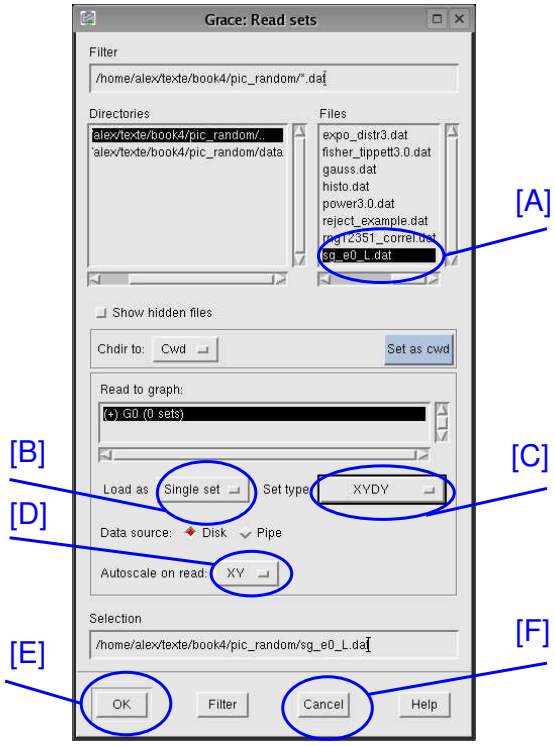


Figure 7.17: The Grace:Read Set window of the *xmgrace* program. Among others, you can select a file [A], choose the type of the input file [B], choose the format of the data [C], what axes should be rescaled automatically on input [D]. You can actually load the data by hitting on the OK button [E] and closing the window by hitting on the Cancel button [F].

shown in the main window (see Fig. 7.18). The axis ranges have been adjusted to the data, because the "Autoscale on read" is set by default to "XY" [D]. You can quickly change the part of the data shown by the buttons (magnifier, AS, Z, z, $\leftarrow$, $\rightarrow$, $\downarrow$, $\uparrow$) on the left of the main window just below the Draw button.

Note that another important input file type is "Block data" where the files consist of many columns of which you only want to show some. When you hit th OK button [E], another window (Grace:Edit block data) will pop up, where you have to select the columns which you actually want to display. For the data format (also when loading block data), some other important choices are XY (no error bars) and XYDYDY (full confidence interval, maybe non-symmetric). Finally, you can close the file selection window, by hitting on the Cancel button [F]. The OK and Cancel buttons are common to all *xmgrace* windows and will not be mentioned explicitly in the following.

In the form the loaded data is shown by default, it is not suitable for publi-

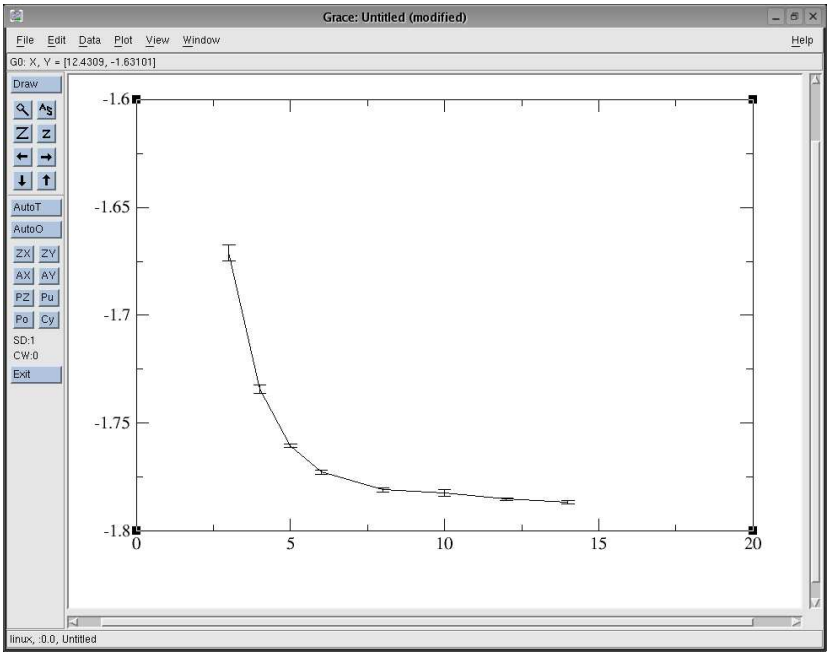


Figure 7.18: The main *xmgrace* window after the data set has been loaded (with auto scale).

cation purposes, because the symbols, lines and fonts are usually too small/ too thin. To adjust many details of your graph, you should go to the Plot menu. First, you choose the Plot appearance... sub menu. A corresponding window will pop up. Here, you should just unselect the "**Fill**" toggle box (upper right corner), because otherwise the bounding box included in the `.eps` file will not match the plot and your figure will overwrite other parts of e.g. your manuscript. The fact that your plot has no background now becomes visible through the appearance of some small dots in the main *xmgrace* window, but this does not disrupt the output when exporting to `.eps`.

Next, you choose the Set appearance... sub menu from the Plot menu. The corresponding window will pop up, see Fig. 7.19. You can pop this window also by double-clicking inside the graph. This window allows to change the actual display style of the data. You have to select the data set or sets [A] to which the changes will be be applied to when hitting the Apply button at the lower left of the window. Note that the list of sets in this box will contain several sets if you have imported more than one data set. Each of them can have (and usually should) its own style. The box where the list of sets appears is also used to administrate the sets. If you hit the right mouse button, while the mouse pointer is inside this box, a menu will pop up, where you can for instance copy or delete sets, hide or unhide them, or rearrange them.

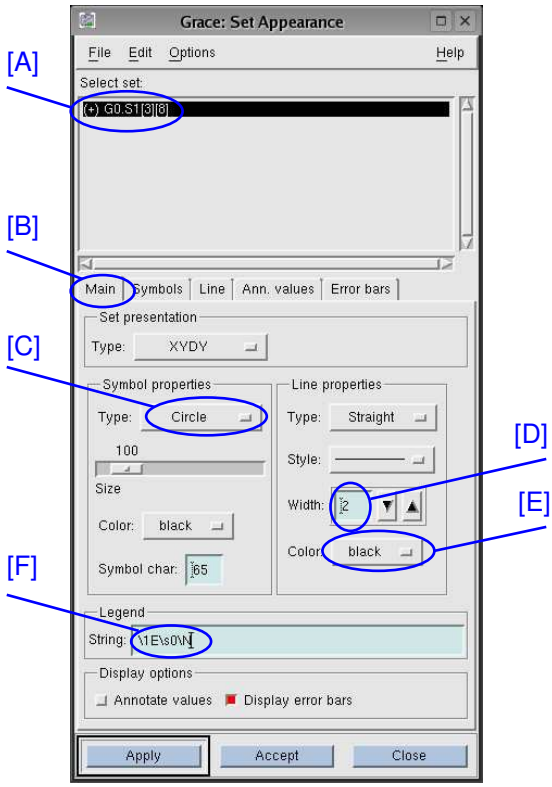


Figure 7.19: The Grace:Set Appearance window of the *xmgrace* program. First you have to select the set or sets which should be addressed by the changes [A]. Due to the large amount of adjustable parameters, the window is organized into different tabs. The most import one is "Main" [B], which is shown here. Among others, you can select a symbol type [C] (below: symbol size, symbol color), choose the width of the lines [D] (also: line type, style) and the color [E]. Furthermore, the label for this data appearing in the legends can be states [F].

The options in this window are arranged within different tabs, the most important is the "Main" tab [B]. Here you can choose whether you want to show symbols for your data points and which type [C], also the symbol sizes and colors. If you want to show lines as well (Line properties area at the right), you can choose the style like "straight" and others, but also "none" is no lines should be displayed. The style can be full, dotted, dashed, and different dotted-dashed styles. For presentations and publications it is important that lines are well visible, in this example a line width of 2 is chosen [D] and a black color [E]. For presentations you can distinguish different data sets also by different colors, but for publications in scientific journals you should keep in mind that the figures are usually printed in black and white, hence light colors are not

visible.[11]

Each data set can have a legend (see below how to activate it). Here, the legend string can be stated. You can enter it directly, with the help of some formatting commands which are characters preceded by a backslash \ . The most important ones are

- \\ prints a backslash.
- \0 selects the Roman font, which is also the default font. A font is active until a new one is chosen.
- \1 selects the *italic* font, used in equations.
- \x selects a symbol font, which contains e.g. Greek characters. For example \xabchqL will generate $\alpha\beta\chi\eta\theta\Lambda$, just to mention some important symbols.
- \s generates a subscript, while \N switches back to normal. For example \xb\s2\N\1(x) generates $\beta_2(x)$.
- \S generates a superscript, for instance \1A\S3x\N-5 generates $A^{3x} - 5$.
- The font size can be changed with \+ and \-.
- With \o and \O one can start and stop overlining, respectively, for instance \1A\oBC\OD generates $A\overline{BC}D$. Underlining can be controlled via \u and \U.

By default, error bars are shown (toggle box lower right corner). At least you should increase the line width for the symbols (Symbols tab) and increase the base and rise line widths for error bars (Error bars tab).

You should know that, when you are creating another plot, you do not have to redo all these and other adjustments of styles. Once you have found your standard, you can save it using the Save Parameters... sub menu from the Plot menu. You can conversely load a parameter set via the Load Parameters... sub menu of the same menu.

Next, you can adjust the properties of the axes, by choosing the Set appearance... sub menu from the Plot menu or by double-clicking on an axis. The corresponding window will pop up, see Fig. 7.20. You have to select the axis where the current changes apply to [A]. For the x axis you should set the range in the fields **Start** [B] and **Stop** [C], here to the values 1 and 15. Below these two fields you find the important Scale field, where you can choose linear scaling (default), logarithmic or reciprocal, to mention the important ones.

The most important adjustments you can perform within the Main tab [D]. Here you enter the label shown below the axis in the Label string field [E]. The format of the string is the same as for the data set legends. Here you enter just

[11] Acting as referee reading scientific papers submitted to journals, I experienced many times that I could not recognize or distinguish some data because they were obviously printed in a light color, or with a thin line width, or with tiny symbols ....

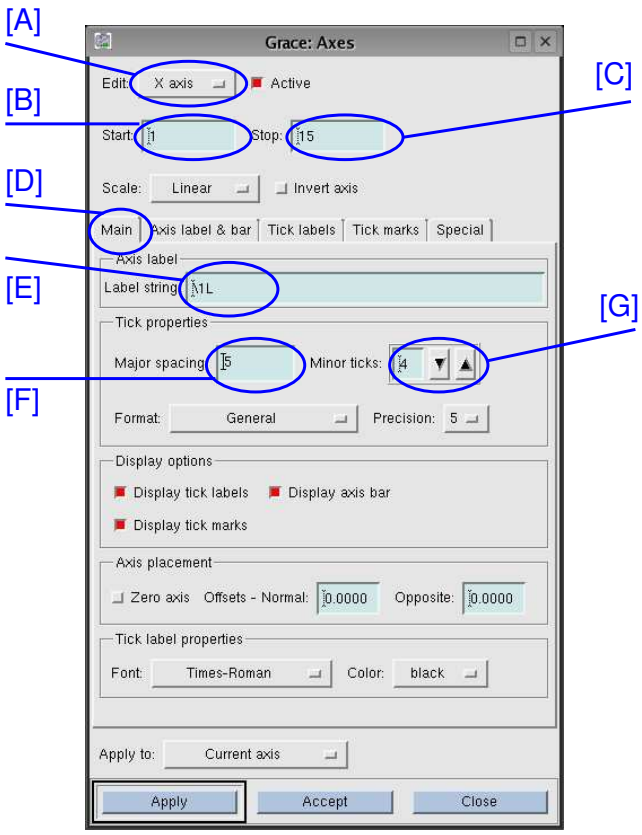


Figure 7.20: The Grace: Axes window of the *xmgrace* program. First you have to select the axis which should be addressed by the changes [A]. Among others, you can change the range in the **Start** [B] and **Stop** [C] fields. Here the Main tab [D] is shown. You can enter an axis label in the Label string field [E] and select the spacing of the major and minor ticks [F,G]

`\1L`, which will show as L. The major spacing of the major (with labels) and minor ticks can be chosen in the corresponding fields [F,G]. Below there is a Format field, where you can choose how the tick labels are printed. Among the many formats, the most common are General ($1, 5, 10, \ldots$), Exponential (`1.0e+00`, `5.0e+00`, `1.0e+01`,...), and Power, which is useful for logarithmic scaled axes ($10^1, 10^2, 10^3, \ldots$). For the tick labels, you can also choose a Precision. This and other fields of this tab you can leave at their standard values here. Nevertheless, you should also adjust the Char size of the axis labels (tab Axis label & bar) and of the tick labels (tab Tick labels). For publications, character sizes above 150% are usually well readable. Note that in the Axis label & bar tab, there is a field Axis transform where you can enter formulas to transform the axis more

or less arbitrarily, see the manual for details. All tabs have many other fields, which are useful as well, but here we stay with the standard choices. Note that sometimes the Special tab is useful, where you can enter all major and minor ticks individually.

To finish the design of the axes, you can perform similar changes to the y axis, with Start field -1.8, Stop field -1.6, Label string field `\1E\s0\N(L)` and the same character sizes as for the x axis for axis labels and tick labels in the corresponding tabs. Note that the axis label will be printed vertically. If you do not like this, you can choose the Perpendicular to axis orientation in the Layout field of the Axis label & bar tab.

Now you have already a nice graph. To show you some more of the capabilities of *xmgrace*, we refine it a bit. Next, you generate an inset, i.e. a small subgraph inside the main graph. This is quite common in scientific publications. For this purpose, you select the underlineEdit menu and there the Arrange graph... sub menu. The corresponding window appears. We want to have just one inset, i.e. in total 2 graphs. For this purpose, you select in the Matrix region of the window the Cols: field to 1 and the Rows: field to 2. Then you hit on the Accept button which applies the changes and closes the window. You now have two graphs, one containing the already loaded data, the other one being empty. These two graphs are currently shown next to each other, one at the top and one at the bottom.

To make the second graph an inset of the first, you choose the Graph appearance... sub menu from the Plot menu. At the top a list of the available graphs is shown [A]. Here you select the first graph `G0`. You need only the Main tab [B], other tabs are for changing styles of titles, frames and legends. We recommend to choose Width 2 in the Frame tab. In the Main tab, you can choose the Type of graph [C], e.g. XY graph, which we use here (default), Polar graph or Pie chart. You only have to change the Viewport coordinates [D] here. These coordinates are relative coordinates, i.e. the standard full viewport including axes, labels and titles is $[0,1] \times [0,1]$. For the main graph `G0`, you choose Xmin and Ymin 0.15 and Xmax and Ymax 0.85. Note that below there is a toggle box Display legend [E], where you can control whether a legend is displayed. If you want to have a legend, you can control its position in the Leg. box tab. Now the different graphs overlap. This does not bother you, because next you select graph `G1` in the list at the top of the window. We want to have the inset in the free area of the plot, in the upper right region. Thus, you enter the viewport coordinates Xmin 0.38, Ymin 0.5, Xmax 0.8 and Ymax 0.8.

Now the second graph is well placed, but empty. We want to show a scaled version of the data in the inset. Hence, you import the data again in the same way as explained above, while choosing Read to graph `G1` in the Grace: Read sets window. In Sec. 7.6.2, you will see that the data follows approximately a power law behavior $e_0(L) = e_\infty + aL^b$ with $e_\infty \approx -1.788$, $a \approx 2.54$ and $b \approx -2.8$. To visualize this, we want to show $e_0(L) - e_\infty$ as a function of L^b. Hence, we want to *transform* the data. You choose from the Data menu the Transformations sub menu and there the Evaluate expression sub sub menu. Note that here you can also find many other transformations, e.g. Fourier transform,

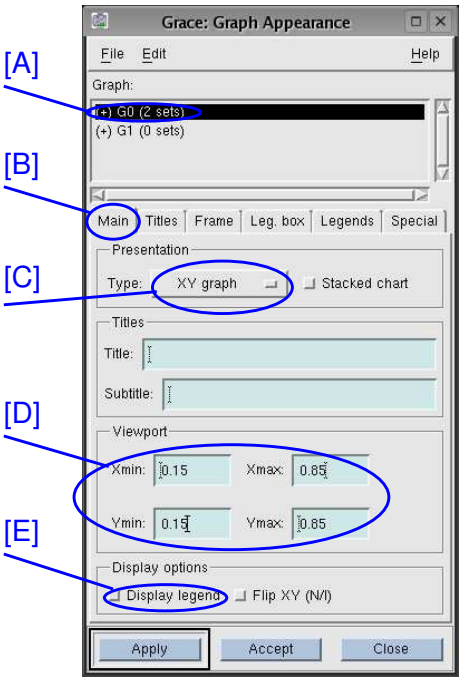


Figure 7.21: The Grace: Graph Appearance window of the *xmgrace* program. At the top one can select to which graph changes should apply [A]. The window is divided into different tabs [B], here the Main tab is shown. The Type of the graph can be selected [C], also Title and Subtitle (empty here). The extensions of the graph can be selected in the Viewport area [D]. This allows to make one graph an inset of another. Using the Display legend toggle [E] the legend can be switched on and off.

interpolation and curve fitting. Please consult the manual for details. In this case, the evaluateExpression window pops up, see Fig. 7.22 (if you did not close the windows you have used before, your screen will be already pretty populated). A transformation always takes the data points from one *source* set, applies a formula to all data points (or to a subset o points) and stores the result in a *destination* set. These sets can be selected at the top of the window in the Source [A] and Destination [B] fields for graph and set separately. Note that the data in the destination set is overwritten. If you want to write the transformed data to a new set, you can first copy an existing set (click on the right mouse button in the Destination Set window and choose Duplicate). In our case, we want to replace the data, hence you select for source and destination the data set from graph `G1`. The transformation is entered below [C], here you first enter `y=y+1.788` to shift the data. The you hit the Apply button at the bottom. Next you change the transformation to `x=x^(-2.8)` and hit the Apply button again.

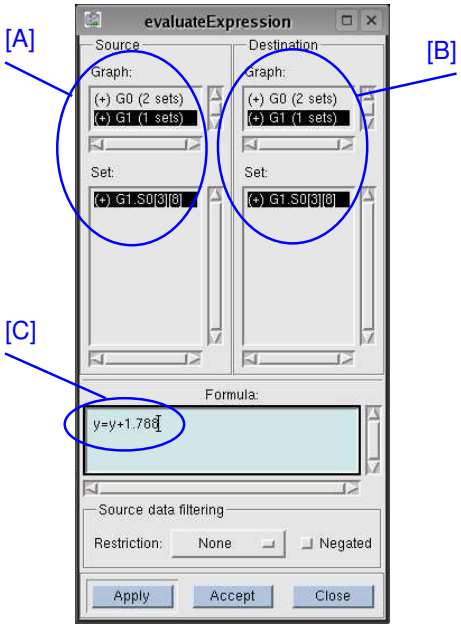


Figure 7.22: The evaluateExpression window of the *xmgrace* program. At the top you can select Source [A] and Destination [B] sets of the transformation. The actual transformation is entered at the bottom [C].

When you now select the second graph by clicking into it, and hit the AS (auto scale) button on the left of the main window, you will see that the data points follow a nice straight line in the inset, which confirms the behavior of the data.

Again you should select symbols, line stiles, and axis labels for the inset. Usually smaller font sizes are used here. Note that all operations always apply to the *current* graph, which can be selected for example by clicking near the corners of the boundary boxes of the graph (which does not always work, depending on which other windows are open) or by double clicking on the corresponding graph in the graph list in the Grace: Graph Appearance window. The final main window is shown in Fig. 7.23. Note that the left axis label is not fully visible. This is no problem when exporting the file as encapsulated postscript; everything will be shown. But if you do not like it, you can adjust the Xmin value of graph G0.

Finally, if you choose the menu Window and the sub menu Drawing objects a window will pop up which enable many graphical elements like texts, lines, boxes and ellipses (again with a variety of choices for colors, styles, sizes etc.) tobe added/changed and deleted in your plot. We do not go into details here.

Now you should save your plot using the File menu and the Save as... sub menu, e.g. with file name `sg_e0_L.agr`, where `.agr` is the typical postfix of *xmgrace* source files. When

GET SOURCE CODE
DIR: `randomness` FILE(S): `sg_e0_L.dat`

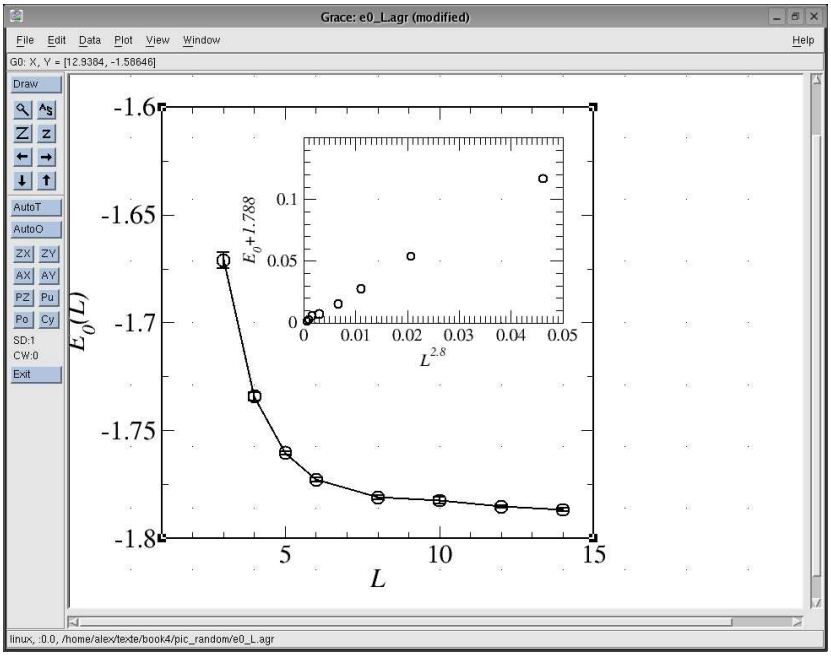


Figure 7.23: The main *xmgrace* window after all adjustments have been made.

you want to create another plot with similar layout later, it is convenient to start from this saved file by copying it to a new file and subsequently using again *xmgrace* to modify the new file.

To export your file as encapsulated postscript, suitable for including it into presentations or publications (see Sec. 8.3), you have to choose the File menu and the Print setup... sub menu. In the window, which pops up, you can select the Device EPS. The file name will automatically switch to `sg_e0_L.eps` (this seems not to work always, in particular if you edit several files, one after the other, please check the file names always). Having hit on the Accept button, you can select the File menu and the Print sub menu, which will generate the desired output file.[12]

Now you have a solid base for viewing and plotting, hence we can continue with advanced analysis techniques. You can experiment with plotting using *xmgrace* in exercise (5).

[12] Using the tool `epstopdf` you can convert the postcript file also to a *pdf* file. With other tools like *convert* or *gimp* you can convert to many other styles.

7.5 Hypothesis testing and (in-)dependence of data

In the previous section, you have learned how to visualized data, mainly data resulting from the basic analysis methods presented in Sec. 7.3. In this section, we proceed with more elaborate analysis methods. One important way to analyze data of simulations is to test hypotheses concerning the results. The hypothesis to be tested is usually called *null hypothesis* H_0. Examples for null hypotheses are:

(A) In a traffic system, opening a new track will decrease the mean value of the travel time $\overline{t}_{\mathrm{A}\to\mathrm{B}}$ for a connection A→B below a target threshold t_{target}.

(B) Within an acquaintance network, a change of the rules describing how people meet will change the distribution of the number of people each person knows.

(C) The distribution of ground-states energies in disordered magnets follows a Fisher-Tippett distribution.

(D) Within a model of an ecological system, the population size of foxes is dependent on the population size of beetles.

(E) For a protein dissolved in water at room temperature, adding a certain salt to the water changes the structure of the protein.

One now can model these situations and use simulations to address the above questions. The aim is to find methods which tell us whetheror not, depending on the results of the simulations, we should *accept* a null hypothesis. There is no general approach. The way we can test H_0 depends on the formulation of the null hypothesis. In any case, our result will again be based on a set of measurements, such as a sample of independent data points $\{x_0, x_1, \ldots, x_{n-1}\}$, formally obtained by sampling from random variables $\{X_0, X_1, \ldots, X_{n-1}\}$ (here again, all described by the same distribution function F_X). To get a solid statistical interpretation, we use a *test statistics*, which is a function of the sample $t = t(x_0, x_1, \ldots, x_{n-1})$. Its distribution describes a corresponding random variable T. This means, you can use any estimator (see page 27), which is also a function of the sample, as test statistics. Nevertheless, there are many test statistics, which usually are not used as estimators.

To get an idea of what a test statistics t may look like, we discuss now test statistics for the above list of examples. For (A), one can use obviously the sample mean. This has to be compared to the threshold value. This will be performed within a statistical interpretation, enabling a null hypothesis to be accepted or rejected, see below. For (B) one needs to compare the distributions of the number of acquaintances before and after the change, respectively. Comparing two distributions can be done in many ways. One can just compare some moments, or define a distance between them based on the difference in

area between the distribution function, just to mention two possibilities. For discrete random variables, the mean-squared difference is particularly suitable, leading to the so-called chi-squared test, see Sec. 7.5.1. For the example (C), the task is similar to (B), only that the empirical results are compared to a given distribution and that the corresponding random variables are continuous. Here, a method based on the maximum distance between two distribution functions is used widely, called Kolmogorov-Smirnov (KS) test (see Sec. 7.5.2). To test hypothesis (D), which means to check for statistical independence, one can record a two-dimensional histogram of the population size of foxes and beetles. This is compared with the distribution where both populations are assumed to be independent, i.e. with the product of the two single-population distribution functions. Here, a variant of the chi-squared test is applied, see Sec. 7.5.3. In the case (E), the sample is not a set of just one-dimensional numbers, instead the simulation results are conformations of proteins given by $3N-$dimensional vectors of the positions $\underline{r}_i$ $(i = 1, \ldots, N)$ of N particles. Here, one could introduce a method to compare two protein conformations $\{\underline{r}_i^A\}$, $\{\underline{r}_i^B\}$ in the following way: First, one "moves" the second protein towards the first one such that the positions of the center of masses agree. Second, one considers the axes through the center of masses and through the first atoms, respectively. One rotates the second protein around its center of mass such that these axes become parallel. Third, the second protein is rotated around the above axis such that the distances between the last atoms of the two proteins are minimized. Finally, for these normalized positions $\{\underline{r}_i^{B\star}\}$, one calculates the squared difference of all pairs of atom positions $d = \sum_i (\underline{r}_i^A - \underline{r}_i^{B\star})^2$ which serves as test function. For a statistical analysis, the distribution of d for one thermally fluctuating protein can be determined via a simulation and then compared to the average value observed when changing the conditions. We do not go into further details here.

The general idea to test a null hypothesis using a test statistics in a statistical meaningful way is as follows:

1. You have to know, at least to an approximate level, the probability distribution function F_T of the test statistics *under the assumption that the null hypothesis is true*. This is the main step and will be covered in detail below.

2. You select a certain significance level α. Then you calculate an interval $[a_l, a_u]$ such that the cumulative probability of T outside the interval equals to α, for instance by distributing the weight equally outside the interval via $F(a_l) = \alpha/2$, $F(a_u) = 1 - \alpha/2$. Sometimes one-sided intervals are more suitable, e.g. $[\infty, a_u]$ with $F(a_u) = 1 - \alpha$, see below concerning example (A).

3. You calculate the actual value t of the test statistics from your simulation. If $t \in [a_l, a_u]$ then you *accept* the hypothesis, otherwise you reject it. Correspondingly, the interval $[a_l, a_u]$ is called *acceptance interval*.

Since this is a probabilistic interpretation, there is a small probability α that you do not accept the null hypothesis, although it is true. This is called a *type*

I error (also called *false negative*), but this error is under control, because α is known.

On the other hand, it is important to realize that in general the fact that the value of the test statistics falls inside the acceptance interval does *not* prove that the null hypothesis is true! A different hypothesis H_1 could indeed hold, just your test statistics is not able to discriminate between the two hypotheses. Or, with a small probability β, you might obtain some value for the test statistics which is unlikely for H_1, but likely for H_0. Accepting the null hypothesis, although it is not true, is called a *type II error* (also called *false positive*). Usually, H_1 is not known, hence β cannot be calculated explicitly. The different cases and the corresponding possibilities are summarized in Fig. 7.24. To conclude: If you want to prove a hypothesis H (up to some confidence level $1-\alpha$), it is better to use the opposite of H as null hypothesis, if this is possible.

reality / test decision	H_0 is true	H_1 is true
accept H_0	correct decision $1-\alpha$	type II error β
reject H_0	type I error α	correct decision $1-\beta$

Figure 7.24: The null hypothesis H_0 might be true, or the alternative (usually unknown) hypothesis H_1. The test of the null hypothesis might result in an acceptance or in a rejection. This leads to the four possible scenarios which appear with the stated probabilities.

Indeed, in general the null hypothesis must be suitably formulated, such that it can be tested, i.e. such that the distribution function F_T describing T can be obtained, at least in principle. For example (A), since the test statistics T is a sample mean, it is safe to assume a Gaussian distribution for T: One can perform enough simulations rather easily, such that the central limit theorem applies. We use as null hypothesis the opposite of the formulated hypothesis (A). Nevertheless, it is impossible to calculate an acceptance interval for the Gaussian distribution based on the assumption that the mean is *larger* than a given value. Here, one can change the null hypothesis, such that instead an expectation value *equal to* t_{target} is assumed. Hence, the null hypothesis assumes that the test statistics has a Gaussian distribution with expectation value t_{target}. The variance of T is unknown, but one can use, as for the calculation of error bars, the sample variance s^2 divided by $n-1$. Now one calculates on this basis an interval $[a_l, \infty]$ with $F_T(a_l) = \alpha$. Therefore, one rejects the null hypothesis if $t < a_l$, which happens with probability α. On the other hand, if the true expectation value is even larger than t_{target}, then the probability of finding a

mean with $t < a_l$ becomes even smaller than α, i.e. less likely. Hence, the hypothesis (A) can be accepted or rejected on the basis of a fixed expectation value.

For a general hypothesis test, to evaluate the distribution of the test statistics T, one can perform a *Monte Carlo simulation*. This means one draws repeatedly samples of size n according to a distribution F_X determined by the null hypothesis. Each time one calculates the test statistics t and records a histogram of these values (or a sample distribution function $F_{\hat{T}}$) which is an approximation of F_T. In this way, the corresponding statistical information can be obtained. To save computing time, in most cases no Monte Carlo simulations are performed, but some knowledge is used to calculate or approximate F_T.

In the following sections, the cases corresponding to examples (B), (C), (D) are discussed in detail. This means, it is explained how one can test for equality of discrete distributions via the chi-squared test and for equality of continuous distributions via the KS test. Finally, some methods for testing concerning (in-)dependence of data and for quantifying the degree of dependence are stated.

7.5.1 Chi-squared test

The chi-squared test is a method to compare histograms and discrete probability distributions. The test works also for discretized (also called *binned*) continuous probability distributions, where the probabilities are obtained by integrating the pdf over the different bins. The test comes in two variants:

- Either you want to compare the histogram $\{h_k\}$ for bins B_k (see Sec. 7.3.3) describing the sample $\{x_0, x_1, \ldots, x_{n-1}\}$ to a given discrete or discretized probability mass function with probabilities $\{p_k\} = P(x \in B_k)$. The null hypothesis H_0 is: "*the sample follows a distribution given by* $\{p_k\}$*"*.

  Note that the probabilities are fixed and independent of the data sample. If the probabilities are parametrized and the parameter is determined by the sample (e.g. by the mean of the data) such that the probabilities fit the data best, related methods as described in Sec. 7.6.2 have to be applied.

- Alternatively, you want to compare two histograms $\{h_k\}$, $\{\hat{h}_k\}$ obtained from two different samples $\{x_0, x_1, \ldots, x_{n-1}\}$ and $\{\hat{x}_0, \hat{x}_1, \ldots, \hat{x}_{n-1}\}$ defined for the same bins B_k. The null hypothesis H_0 is: "*the two samples follow the same distribution*".[13]

In case the test is used to compare intrinsically discrete data, the intervals B_k can conveniently be chosen such that each possible outcome corresponds to one interval. Note that due to the binning process, the test can be applied to high-dimensional data as well, where the sample is a set of vectors. Also non-numerical data can be binned. In these cases each bin represents either a subset

[13] Note that here we assume that the two samples have the same size, which is usually easy to achieve in simulations. A different case occurs when also the number of sample points is a random variable, hence a difference in the number of sample points makes the acceptance of H_0 less likely, see [Press et al. (1995)].

of the high-dimensional space or, in general, a subset of the possible outcomes. For simplicity, we restrict ourselves here to one-dimensional numerical samples.

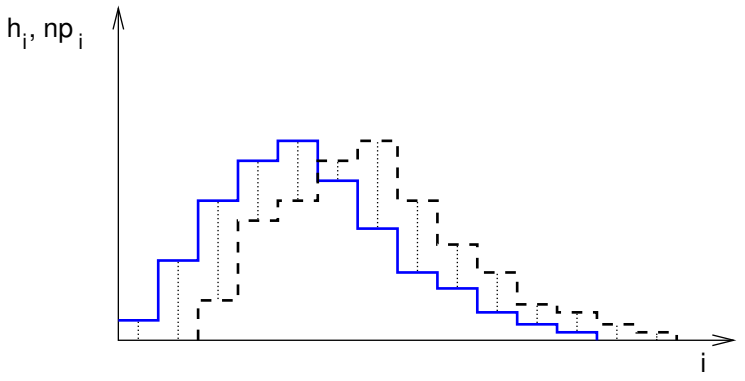


Figure 7.25: Chi-squared statistics: A histogram (solid line) is compared to a discrete probability distribution (dashed line). For each bin, the sum of the squared differences of the bin counter h_k to the expected number of counts np_k is calculated (dotted vertical lines), see Eq. (7.68). In this case, the differences are quite notable, thus the probability that the histogram was obtained via random experiments from a random variable described by the probabilities $\{p_k\}$ (null hypothesis) will be quite small.

We start with the first case, where a sample histogram is compared to a probability distribution, corresponding to example (C) on page 57. The test statistics, called χ^2, is defined as:

$$\chi^2 = \sum_k{}' \frac{(h_k - np_k)^2}{np_k} \tag{7.68}$$

with np_k being the expected number of sample points in bin B_k. The prime at the sum symbol indicates that bins with $h_k = np_k = 0$ are omitted. The number of contributing bins is denoted by K'. If the pmf p_k is nonzero for an infinite number of bins, the sum is truncated for terms $np_k \ll 1$. This means that the number of contributing bins will be always finite. Note that bins exhibiting $h_k > 0$ but $p_k = 0$ are not omitted. This results in an infinite value of χ^2, which is reasonable, because for data with $h_k > 0$ but $p_k = 0$, the data cannot be described by the probabilities p_k.

The chi-squared distribution with $\nu = K' - 1$ degrees of freedom (see Eq. (7.45)) describes the chi-squared test statistics, if the number of bins and the number of bin entries is large. The term -1 in the number of degrees of freedom comes from the fact that the total number of data points n is equal to the total number of expected data points $\sum_k n_k p_k = n \sum_k p_k = n$, hence the K' different summands are not statistically independent. The probability density of the chi-squared distribution is given in Eq. (7.45). To perform the actual test, it is

recommended to use the implementation in the *GNU scientific library* (GSL) (see Sec. 6.3).

GET SOURCE CODE
DIR: `randomness` FILE(S): `chi2.c`

Next, a C function `chi2_hd()` is shown which calculates the cumulative probability (*p-value*) that a value of χ^2 or larger is obtained, given the null hypothesis that the sample was generated using the probabilities p_k. Arguments of `chi2_hd()` are the number of bins, and two arrays `h[]` and `p[]` containing the histogram h_k and the probabilities p_k, respectively:

```
1  double chi2_hd(int n_bins, int *h, double *p)
2  {
3    int n;                       /* total number of sample points */
4    double chi2;                                 /* chi^2 value */
5    int K_prime;                  /* number of contributing bins */
6    int i;                                        /* counter */
7
8    n = 0;
9    for(i=0; i<n_bins; i++)
10     n += h[i];      /* calculate total number of sample_points */
11
12   chi2 = 0.0; K_prime = 0;
13   for(i=0; i<n_bins; i++)                  /* calculate chi^2 */
14   {
15     if(p[i] > 0)
16     {
17       chi2 += (h[i]-n*p[i])*(h[i]/(n*p[i])-1.0);
18       K_prime ++;
19     }
20     else if(h[i] >0)       /* bin entry for zero probability ? */
21     {
22       chi2 = 1e60;
23       K_prime ++;
24     }
25   }
26   return(gsl_cdf_chisq_Q(chi2, K_prime-1));
27 }
```

First, in lines 8–10, the total number of sample points is obtained from summing up all histogram entries. In the main loop, lines 12–25, the value of χ^2 is calculated. In parallel, the number of contributing bins is determined. Finally (line 26) the p-value is obtained using the GSL function `gsl_cdf_chisq_Q()`. This p-value can be compared with the significance level α. If the the p-value is larger, the null hypothesis is accepted, otherwise rejected.

Note that the result for the p-value clearly depends on the number of bins, and, if applicable, on the actual choice of bins. Nevertheless, all reasonable choices, although maybe leading to somehow different numerical results, will lead to the same decisions concerning the null hypothesis in most cases.

Next, we consider the case, where we want to compare two histograms $\{h_k\}, \{\hat{h}_k\}$ corresponding to example (B) on page 57. In this case the χ^2 statistics reads

$$\chi^2 = \sum_k{}' \frac{(h_k - \hat{h}_k)^2}{h_k + \hat{h}_k} \tag{7.69}$$

The sum runs over all bins where $h_k \neq 0$ or $\hat{h}_k \neq 0$, and K' being the corresponding number of contributing bins. Consequently, the bins which should be included are uniquely defined, in contrast to the case where a histogram is compared to a distribution defined for infinitely many outcomes. Note that in the denominator the sum of the bin entries occurs, not the average. The reason is that the chi-squared distribution is a sum of standard Gaussian distributed numbers (variance 1) and here, where the differences of two (approximately) Gaussian quantities are taken, the resulting variance is the sum of the individual variances, approximated roughly by the histogram entries. To calculate the p-value, again the chi-squared distribution with $\nu = K' - 1$ degrees of freedom is to be applied. Here, no C implementation is shown, rather we refer the reader to exercise (6).

7.5.2 Kolmogorov-Smirnov test

Next, we consider the case where the statistical properties of a sample $\{x_0, x_1, \ldots, x_{n-1}\}$, obtained from a repeated experiment using a continuous random variable, is to be compared to a given distribution function F_X. One could, in principle, compare a histogram and a correspondingly binned probability distribution using the chi-squared test explained in the previous section. Unfortunately, the binning is artificial and has an influence on the results (imagine few very large bins). Consequently, the method presented in this section is usually preferred, since it requires no binning. Note that if the distribution function is parametrized and if the parameter is determined by the sample (e.g. by the mean of the data) such that the F_X fits the data best, the methods from Sec. 7.6.2 have to be applied.

The basic idea of the *Kolmogorov-Smirnov* test is to compare the distribution function to the empirical sample distribution function $F_{\hat{X}}$ defined in Eq. (7.65). Note that $F_{\hat{X}}(x)$ is piecewise constant with jumps of size $1/n$ at the positions x_i (assuming that each data point is contained uniquely in the sample).

Here again, one has several choices for the test statistics. For instance, one could calculate the area between F_X and $F_{\hat{X}}$. Instead, usually just the maximum difference between the two functions is used:

$$d_{\max} \equiv \max_x \left| F_X(x) - F_{\hat{X}}(x) \right| \tag{7.70}$$

Since the sample distribution function changes only at the sample points, one has to perform the comparison just before and just after the jumps. Thus, Eq. (7.70) is equivalent to

$$d_{\max} \equiv \max_{x_i} \left\{ \left| F_X(x_i) - 1/n - F_{\hat{X}}(x_i) \right|, \left| F_X(x_i) - F_{\hat{X}}(x_i) \right| \right\}$$

This sample statistics is visualized in Fig. 7.26.

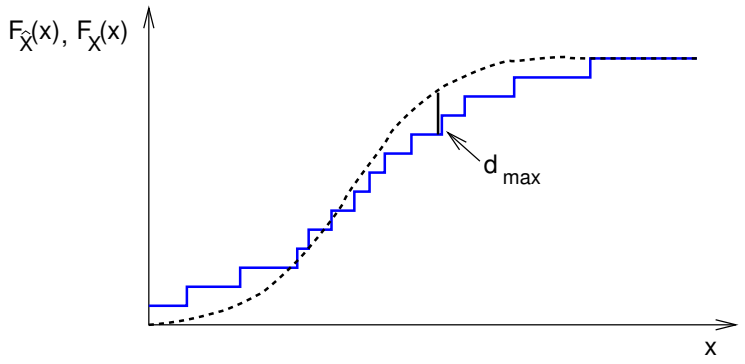


Figure 7.26: Kolmogorov-Smirnov test: A sample distribution function (solid line) is compared to a given probability distribution function (dashed line). The sample statistics $d_{\max}$ is the maximum difference between the two functions.

The p-value, i.e. the probability of a value of $d_{\max}$ as measured ($d_{\max}^{\text{measured}}$) or worse, given the null hypothesis that the sample is drawn from F_X, is approximately given by (see [Press et al. (1995)] and references therein):

$$P(d_{\max} \geq d_{\max}^{\text{measured}}) = Q_{\text{KS}}\left([\sqrt{n} + 0.12 + 0.11/\sqrt{n}] d_{\max}^{\text{measured}} \right) \tag{7.71}$$

This approximation is already quite good for $n \geq 8$. Here, the following auxiliary probability function is used:

$$Q_{\text{KS}}(\lambda) = 2 \sum_{i=1}^{\infty} (-1)^{i+1} e^{-2i^2\lambda^2} \tag{7.72}$$

with $Q_{\text{KS}}(0) = 1$ and $Q_{\text{KS}}(\infty) = 0$. This function can be implemented most easily by a direct summation [Press et al. (1995)]. The function `Q_ks()` receives the value of λ as argument and returns $Q_{\text{KS}}(\lambda)$:

GET SOURCE CODE
DIR: `randomness` FILE(S): `ks.c`

```
1  double Q_ks(double lambda)
2  {
3    const double eps1 = 0.0001;  /* relative margin for stop */
4    const double eps2 = 1e-10;   /* relative margin for stop */
5    int i;                                  /* loop counter */
6    double sum;                              /* final value */
7    double factor;           /* constant factor in exponent */
```

```
8   double sign;                                /* of summand */
9   double term, last_term;        /* summands, last summand */
10
11  sum = 0.0; last_term = 0.0; sign = 1.0;    /* initialize */
12  factor = -2.0*lambda*lambda;
13  for(i=1; i<100; i++)                           /* sum up */
14  {
15    term = sign*exp(factor*i*i);
16    sum += term;
17    if( (fabs(term) <= eps1*fabs(last_term)) ||
18        (fabs(term) <= eps2*sum))
19      return(2*sum);
20    sign =- sign;
21    last_term = term;
22  }
23  return(1.0);                /* in case of no convergence */
24 }
```

The summation (lines 13–22) is performed for at most 100 iterations. If the current term is small compared to the previous one or very small compared to the sum obtained so far, the summation is stopped (line 17–18). If this does not happen within 100 iterations, the sum has not converged (which means λ is very small) and $Q(0) = 1$ is returned.

This leads to the following C implementation for the KS test. The function `ks()` expects as arguments the number of sample points `n`, the sample `x[]` and a pointer `F` to the distribution function:

```
1  double ks(int n, double *x, double (*F)(double))
2  {
3    double d, d_max;                    /* (maximum) distance */
4    int i;                                   /* loop counter */
5    double F_X;            /* empirical distribution function */
6
7    qsort(x, n, sizeof(double), compare_double);
8
9    F_X = 0; d_max = 0.0;
10   for(i=0; i<n; i++)                   /* scan through F_X */
11   {
12     d = fabs(F_X-F(x[i]));   /* distance before jump of F_X */
13     if( d> d_max)
14       d_max = d;
15     F_X += 1.0/n;
16     d = fabs(F_X-F(x[i]));    /* distance after jump of F_X */
17     if( d> d_max)
18       d_max = d;
19   }
20   return(Q_ks( d_max*(sqrt(n)+0.12+0.11/sqrt(n))));
21 }
```

First the sample is sorted (line 7). This allows for a simple implementation

of the sample distribution function, because at each sample data point, in the order of occurrence, the value of $F_{\hat{X}}$ is increased by $1/n$. When obtaining the maximum distance (lines 10–19), one has to compare $F_{\hat{X}}$ to the distribution function F_X just before (lines 12–14) and after (lines 15–18) the jumps. Note that this implementation works also for samples, where some data points occur multiple times.

For the actual test, one calculates the p-value for the given sample using `ks()`. If the p-value exceeds the indented significance level α, the null hypothesis is accepted, i.e. the data is compatible with the distribution with high probability. Usually quite small significances are used, e.g. $\alpha = 0.05$. This means that even substantial values of $d_{\max}$ are accepted. Thus, one rejects the null hypothesis only, as usual, in case the probability for an error of type I is quite small.

It is also possible to compare two samples of sizes n_1, n_2 via the KS test. The test statistics for the two sample distribution functions is again the maximum distance. The probability to find a value of $d_{\max}$ as obtained or worse, given the null hypothesis that the samples are drawn from the same distribution, is as above in Eq. (7.71), only one has to replace n by the "effective" sample size $n_{\text{eff}} = n_1 n_2/(n_1 + n_2)$, for details see [Press et al. (1995)] and references therein. It is straightforward to implement this test when using the C function `ks()` shown above as template.

7.5.3 Statistical (in-)dependence

Here, we consider samples, which consist of pairs (x_i, y_i) $(i = 0, 1, \ldots, n-1)$ of data points. Generalizations to higher-dimensional data is straightforward. The question is, whether the y_i values depend on the x_i values (or vice versa). In this case, one also says that they are *statistically related*. If yes, this means that if we know one of the two values, we can predict the other one with higher accuracy. The formal definition of statistical (in-) dependence was given in Sec. 7.1. An example of statistical dependence occurs in weather simulations: The amount of snowfall is statistically related to the temperature: If it is too warm or too cold, it will not snow. This also shows, that the dependence of two variables it not necessarily monotonous. In case one is interested in monotonous and even linear dependence, one usually says that the variables are *correlated*, see below.

GET SOURCE CODE

DIR: `randomness`
FILE(S): `points0A.dat`
`points0B.dat`
`points1A.dat`
`points1B.dat`

It is important to realize that we have to distinguish between statistical *significance* of a statistical dependence and the *strength* of the dependence. Say that our test tells us that the x values are statistically related with high probability. This usually just means that we have a large sample. On the other hand, the strength of the statistical dependence can be still small. It could be, for eaxample, that a given value for x will influence the probability distribution for y only slightly. One the other hand, the strength can be large, which means, for example, knowing x almost determines y. But if we have only few samples points, we cannot be

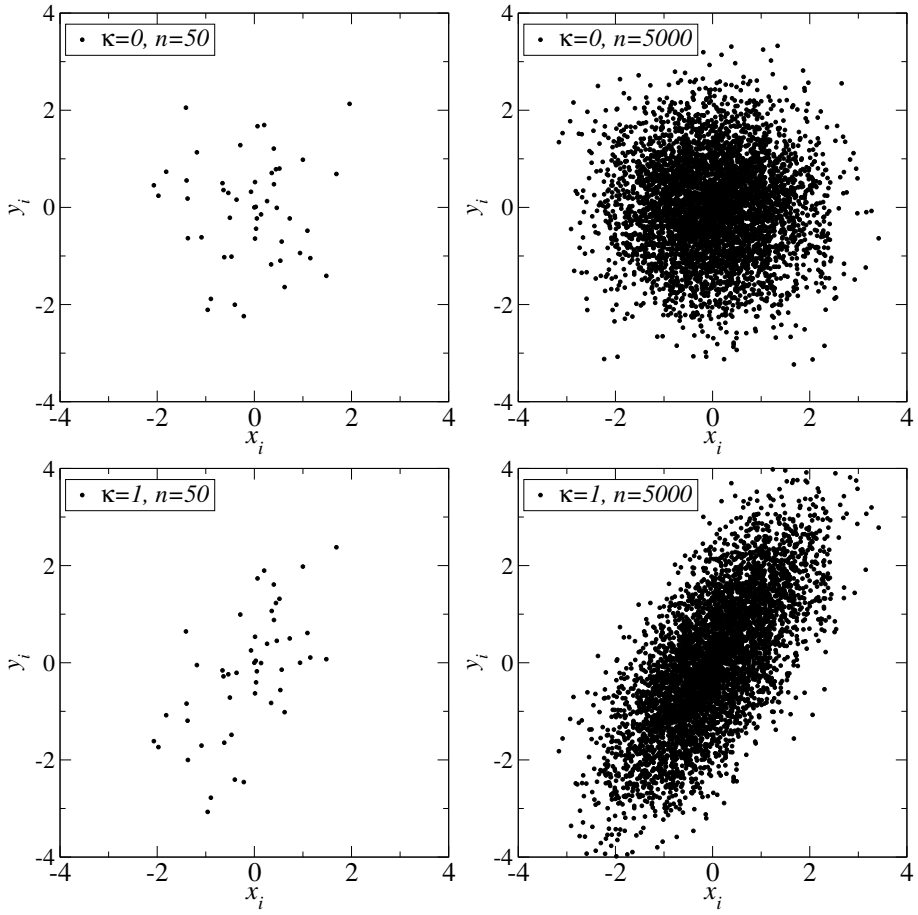


Figure 7.27: Scatter plots for n data points (x_i, y_i) where the x_i numbers are generated from a standard Gaussian distribution (expectation value 0, variance 1), while each y_i number is drawn from a Gaussian distribution with expectation value κx_i (variance 1).

very sure whether the data points are related or not. Nevertheless, there is some connection: the larger the strength, the easier it is to show that the dependence is significant. For illustration consider a sample where the x_i numbers are generated from a standard Gaussian distribution (expectation value 0, variance 1), while each y_i number is drawn from a Gaussian distribution with expectation value κx_i (variance 1).[14] Hence, if $\kappa = 0$, the data points are independent. Scatter plots, where each sample point (x_i, y_i) is shown as dot in the $x-y$ plane

[14]This is an example, where the random variables Y_i which described the sample are not identical.

are exposed in Fig. 7.27. Four possibilities are presented, $k = 0/1$ combined with $n = 50/5000$. Below, we will also present what the methods we use here will tell us about these data sets.

In this section, first a variant of the chi-squared test is presented, which enables us to check whether data is independent. Next, the *linear correlation coefficient* is given, which states the strength of linear correlation. Finally, it is discussed how one can quantify the dependence *within* a sample, for example between sample points $x_i, x_i + \tau$.

To test statistical dependence for a sample $\{(x_0, y_0), (x_1, y_1), \ldots, (x_{n-1}, y_{n-1})\}$, one considers usually the null hypothesis: H_0 = "The x sample points and the y sample points are independent." To test H_0 one puts the pairs of sample points into two-dimensional histograms $\{h_{kl}\}$. The counter h_{kl} receives a count, if for data point (x_i, y_i) we have $x_i \in B_k^{(x)}$ and $y_i \in B_l^{(y)}$, for suitably determined bins $\{B_k^{(x)}\}$ and $\{B_l^{(y)}\}$. Let k_x and k_y the number of bins in x and y direction, respectively. Next, one calculates single-value (or one-dimensional) histograms $\{\hat{h}_k^{(x)}\}$ and $\{\hat{h}_l^{(y)}\}$ defined by

$$\begin{aligned} \hat{h}_k^{(x)} &= \sum_l h_{kl} \\ \hat{h}_l^{(y)} &= \sum_k h_{kl} \end{aligned} \tag{7.73}$$

These one-dimensional histograms describe how many counts in a certain bin arise for one variable, regardless of the value of the other variable. It is assumed that all entries of these histograms are not empty. If not, the bins should be adjusted accordingly. Note that $n = \sum_k \hat{h}_k^{(x)} = \sum_l \hat{h}_l^{(y)} = \sum_{kl} h_{kl}$ holds.

Relative frequencies, which are estimates of probabilities, are obtained by normalizing with n, i.e. $\hat{h}_k^{(x)}/n$ and $\hat{h}_l^{(y)}/n$. If the two variables x_i, y_i are independent, then the relative frequency to obtain a pair of values (x, y) in bins $\{B_k^{(x)}\}$ and $\{B_l^{(y)}\}$ should be the product of the single-value relative frequencies. Consequently, by multiplying with n one obtains the corresponding expected number n_{kl} of counts, under the assumption that H_0 holds:

$$n_{kl} = n \frac{\hat{h}_k^{(x)}}{n} \frac{\hat{h}_l^{(y)}}{n} = \frac{\hat{h}_k^{(x)} \hat{h}_l^{(y)}}{n} \tag{7.74}$$

These expected numbers are compared to the actual numbers in the two-dimensional histogram $\{h_{kl}\}$ via the χ^2 test statistics, comparable to Eq. (7.68):

$$\chi^2 = \sum_{kl} \frac{(h_{kl} - n_{kl})^2}{n_{kl}} \tag{7.75}$$

The statistical interpretation of χ^2 is again provided by the chi-squared distribution. The number of degrees of freedom is determined by the number of bins $(k_x k_y)$ in the two-dimensional histogram minus the number of constraints. The constraints are given by Eq. (7.73), except that the total number of counts

being n is contained twice, resulting in $k_x + k_y - 1$. Consequently, the number of degrees of freedom is

$$\nu = k_x k_y - k_x - k_y + 1 \,. \tag{7.76}$$

Therefore, under the assumption that the x and y sample points are independent, $p = 1 - F(\chi^2, \nu)$ gives the probability (p-value) of observing a test statistics of χ^2 or larger. F is here the distribution function of the chi-square distribution, see Eq. (7.45). This p-value has to be compared to the significance level α. If $p < \alpha$, the null hypothesis is rejected.

The following C function implements the chi-squared independence test `chi2_indep()`. It receives the number of bins in x and y direction as arguments, as well as a two-dimensional array, which carries the histogram:

GET SOURCE CODE
DIR: `randomness` FILE(S): `chi2indep.c`

```
1  double chi2_indep(int n_x, int n_y, int **h)
2  {
3    int n;                       /* total number of sample points */
4    double chi2;                                  /* chi^2 value */
5    int k_x, k_y;                /* number of contributing bins */
6    int k, l;                                       /* counters */
7    int *hx, *hy;                 /* one-dimensional histograms */
8
9    hx = (int *) malloc(n_x*sizeof(int));           /* allocate */
10   hy = (int *) malloc(n_y*sizeof(int));
11
12   n = 0;            /* calculate total number of sample_points */
13   for(k=0; k<n_x; k++)
14     for(l=0; l<n_y; l++)
15       n += h[k][l];
16
17   k_x = 0;                  /* calculate 1-dim histogram for x */
18   for(k=0; k<n_x; k++)
19   {
20     hx[k] = 0;
21     for(l=0; l<n_y; l++)
22       hx[k] += h[k][l];
23     if(hx[k] > 0)                  /* does x bin contribute ? */
24       k_x++;
25   }
26
```

```
27   k_y = 0;                  /* calculate 1-dim histogram for y */
28   for(l=0; l<n_y; l++)
29   {
30     hy[l] = 0;
31     for(k=0; k<n_x; k++)
32       hy[l] += h[k][l];
33     if(hy[l] > 0)                    /* does y bin contribute ? */
34       k_y++;
35   }
36
37   chi2 = 0.0;
38   for(k=0; k<n_x; k++)                       /* calculate chi^2 */
39     for(l=0; l<n_y; l++)
40       if( (hx[k] != 0)&&(hy[l] != 0) )
41         chi2 += pow(h[k][l]-(double) hx[k]*hy[l]/n, 2.0)/
42           ((double) hx[k]*hy[l]/n);
43
44   free(hx);
45   free(hy);
46   return(gsl_cdf_chisq_Q(chi2, k_x*k_y - k_x -k_y + 1));
47 }
```

First, the one-dimensional histograms are allocated (lines 9–10). Then the total number of counts, i.e. the sample size, is calculated (lines 12–15). In lines 17–26, the one-dimensional histogram for the x direction is obtained. Also the effective number of bins in that direction is calculated. In lines 27–35, the same happens for the y direction. The actual value of the χ^2 test statistics is determined in lines 37–42. Finally, the allocated memory is freed (lines 44-45) and the p-value calculated (line 46), again the GSL function `gsl_cdf_chisq_Q()` is used.

The p-values for the sample sets shown in Fig. 7.27 are as follows: $p(\kappa = 0, n = 50) = 0.077$, $p(\kappa = 0, n = 5000) = 0.457$, $p(\kappa = 1, n = 50) = 0.140$, $p(\kappa = 1, n = 5000) < 10^{-100}$. Hence, the null hypothesis of independence would not be rejected (say $\alpha = 0.05$) for the case $\kappa = 1, n = 50$, which is actually correlated. On the other hand, if the number of samples is large enough, there is no doubt.

Once it is established that a sample contains dependent data, one can try to measure the strength of dependence. A standard way is to use the *linear correlation coefficient* (also called *Pearson's* r) given by

$$r \equiv \frac{\sum_i (x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_i (x_i - \overline{x})^2} \sqrt{\sum_i (y_i - \overline{y})^2}} \,. \tag{7.77}$$

This coefficient assumes, as indicated by the name, that a linear correlation exists within the data. The implementation using a C function is straight forward, see exercise (7). For the data shown in Fig. 7.27, the following correlation coefficients are obtained: $r(\kappa = 0, n = 50) = 0.009$, $r(\kappa = 0, n = 5000) = 0.009$, $r(\kappa = 1, n = 50) = 0.653$, $r(\kappa = 1, n = 5000) = 0.701$. Here, also in the two cases, where the statistics is low, the value of r reflects whether or not the data

is correlated. Nevertheless, this is only the case because we compare strongly correlated data to uncorrelated data. If we compare weakly but significantly correlated data, we will still get a small value of r. Hence, to test for significance, it is better to use the hypothesis test based on the χ^2 test statistics.

Finally, note that a different type of correlation may arise: So far it was always assumed that the different sample points x_i, x_j (or sample vectors) are statistically independent of each other. Nevertheless, it could be the case, for instance, that the sample is generated using a Markov chain Monte Carlo simulation [Newman and Barkema (1999), Landau and Binder (2000), Robert and Casella (2004), Liu (2008)], where each data point x_{i+1} is calculated using some random process, but also depends on the previous data point x_i, hence i is a kind of artificial sample time of the simulation. This dependence decreases with growing time distance between sample points. One way to see how quickly this dependence decreases is to use a variation of the correlation coefficient Eq. (7.77), i.e. a *correlation function*:

$$\begin{aligned}\tilde{C}(\tau) &= \frac{1}{n-\tau}\sum_{i=0}^{n-1-\tau} x_i x_{i+\tau} \\ &\quad - \left(\frac{1}{n-\tau}\sum_{i=0}^{n-1-\tau} x_i\right) \times \left(\frac{1}{n-\tau}\sum_{i=0}^{n-1-\tau} x_{i+\tau}\right) \end{aligned} \tag{7.78}$$

The term $\frac{1}{n-\tau}\sum_{i=0}^{n-1-\tau} x_i \times \frac{1}{n-\tau}\sum_{i=0}^{n-1-\tau} x_{i+\tau}$ will converge to $\overline{x}^2$ for $n \to \infty$ if it can be assumed that the distribution of the sample points is stationary, i.e. does not depend on the sample time. Therefore, $\tilde{C}(\tau)$ is approximately $\frac{1}{n-\tau}\sum_{i=0}^{n-1-\tau}(x_i - \overline{x})(x_{i+\tau} - \overline{x})$, comparable to the nominator of the linear correlation coefficient Eq. (7.77). Usually one normalizes the correlation function by $\tilde{C}(0)$, which is just the sample variance in the stationary case, see Eq. (7.51):

$$C(\tau) = \tilde{C}(\tau)/C(0)\,. \tag{7.79}$$

Consequently, for any data, for example obtained from a Markov chain Monte Carlo simulation, $C(0) = 1$ will always hold, Then $C(\tau)$ decreases with increasing difference τ, see for example Fig. 7.28. Very often the functional form is similar to an exponential $\sim \exp(-\tau/\tau_c)$. In theory, $C(\tau)$ should converge to zero for $\tau \to \infty$, but due to the finite size of the sample, usually strong fluctuations appear for τ approaching n. A typical time τ_c which measures how fast the dependence of the sample points decreases is given by $C(\tau_c) = 1/e$, which is consistent with the above expression, if the correlation function decreases exponentially. At twice this distance, the correlation is already substantially decreases (to $1/e^2$). Consequently, if you want to obtain error bars for samples obtained from dependent data, you could include for instance only points $x_0, x_2\tau_c, x_{4\tau_c}, x_{6\tau_c}, \ldots$ in a sample, or just use $n/(2\tau_c)$ instead of n in any calculation of error bars. Although these error bars are different from those if the sample was really independent, it gives a fairly good impression of the statistical error.

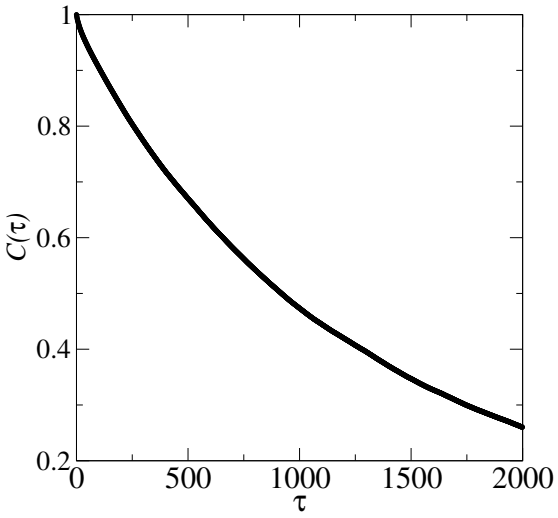


Figure 7.28: Correlation function $C(\tau)$ for a simulation of a ferromagnetic system, x_i being the magnetization at time step i. (For experts: Ising system of size 16×16 spins simulated with single-spin flip Metropolis Monte Carlo at a (reduced) temperature $T = 2.269$ close to the phase transition temperature, where correlation times τ_c are large).

Alternatively, to obtain a typical time τ_c without calculating a correlation function, you can also use the *blocking method* [Flyvbjerg (1998)]. Within this approach, you iteratively merge neighboring data points via $x_i^{(z+1)} = (x_{2i}^{(z)} + x_{2i+1}^{(z)})/2$ and $n^{(z+1)} = n^{(z)}/2$ (iteration level $z = 0$ corresponds to the original sample). You calculate the standard error bar $\sigma^{(z)}/\sqrt{n^{(z)} - 1}$ for each iteration level. Once it reaches a plateau at level z_c, the data is (almost) independent and the true error bar is given by the level value. Then $\tau_c = 2^{z_c}$ is a typical time of independence of the data points.

If you are really just interested in error bars, i.e. you do not need to know the value of τ_c, you could also use the bootstrap approach which is not susceptible to dependence of data, see Sec. 7.3.4.

7.6 General estimators

In Sec. 7.3, different methods are presented of how to estimate parameters which can be obtained directly and simply from the given sample $\{x_0, x_1, \ldots, x_{n-1}\}$. In this section, a general method is considered which enables estimators to be obtained for arbitrary parameters of probability distributions. The method is based on the *maximum-likelihood principle*, which is exposed in Sec. 7.6.1. This principle can be extended to the *modeling of data*, where often a sample of

triplets $\{(x_0, y_0, \sigma_0), (x_1, y_1, \sigma_1), \ \ldots, \ (x_{n-1}, y_{n-1}, \sigma_{n-1})\}$ is given. Typically the x_i data points represent some control parameter, which can be chosen in the simulation, such as the temperature of a gas. It is assumed that all x_i values are different. Consequently, the simulation has been carried out at n different values of the control parameter. The y_i data points are averages of measurements (e.g. the density of the gas) obtained in the simulations for the fixed value x_i of the control parameter. The σ_i values are the corresponding error bars.[15] Modeling the data means that one wants to determine a relationship $y = y(x)$. Usually some assumptions or knowledge about the relationship are available, which means one has available one parametrized test function $y_{\underline{\theta}}(x)$. Consequently, the set of parameters has to be adjusted $\underline{\theta}$ such that the function $y_{\underline{\theta}}(x)$ *fits* the sample "best". This is called *data fitting* and will be explained in Sec. 7.6.2. This approach can also be used to compare several fitted test functions to determined which represents the most suitable model.

7.6.1 Maximum likelihood

Here, we consider the following task: For a given sample $\{x_0, x_1, \ \ldots, \ x_{n-1}\}$ and a probability distribution represented by a pmf $p_{\underline{\theta}}(x)$ or a pdf $f_{\underline{\theta}}(x)$, we want to determine the parameters $\underline{\theta} = (\theta_1, \ldots, \theta_{n_\mathrm{p}})$ such that the pmf or pdf represents the data "best". This is written in parentheses, because there is not unique definition what "best" means, or even a mathematical way to derive a suitable criterion. If one assumes no prior knowledge about the parameters, one can use the following principle:

Definition The *maximum-likelihood principle* states that the parameters $\underline{\theta}$ should be chosen such that the likelihood of the data set, given the parameters, is maximal.

In case of a discrete random variable, if it can be assumed that the different data points are independent, the likelihood of the data is just given by the product of the single data point probabilities. This defines the *likelihood function*

$$L(\underline{\theta}) \equiv p_{\underline{\theta}}(x_1) p_{\underline{\theta}}(x_2) \ldots p_{\underline{\theta}}(x_{n-1}) = \prod_{i=0}^{n-1} p_{\underline{\theta}}(x_i) \tag{7.80}$$

For the continuous case, the probability to obtain during a random experiment exactly a certain sample is zero. Nevertheless, for a small uncertainty parameter ϵ, the probability to obtain a value in the interval $[\tilde{x} - \epsilon, \tilde{x} + \epsilon]$ is $P(\tilde{x} - \epsilon \leq X < \tilde{x} + \epsilon) = \int_{\tilde{x}-\epsilon}^{\tilde{x}+\epsilon} f_{\underline{\theta}}(x)\, dx \approx f_{\underline{\theta}}(\tilde{x}) 2\epsilon$. Since 2ϵ enters just as a factor, it is not relevant to determining the maximum. Consequently, for the continuous case, one considers the following likelihood function

$$L(\underline{\theta}) \equiv f_{\underline{\theta}}(x_1) f_{\underline{\theta}}(x_2) \ldots f_{\underline{\theta}}(x_{n-1}) = \prod_{i=0}^{n-1} f_{\underline{\theta}}(x_i) \tag{7.81}$$

[15] Sometimes also the x_i data points are measured quantities which are also characterized by error bars. The generalization of the methods to this case is straightforward.

To find the maximum of a likelihood function $L(\underline{\theta})$ analytically, one has to calculate the first derivatives with respect to all parameters, respectively, and requires them to be zero. Since calculating the derivative of a product involves the application of the product rule, it is usually more convenient to consider the *log-likelihood function*

$$l(\underline{\theta}) \equiv \log L(\underline{\theta})\,. \tag{7.82}$$

This turns the product of single-data-points pmfs or pdfs into a sum, where the derivatives are easier to obtain. Furthermore, since the logarithm is a monotonous function, the maximum of the likelihood function is the same as the maximum of the log-likelihood function. Hence, the parameters which suit "best" are determined within the maximum-likelihood approach by the set of equations

$$\frac{\partial l(\underline{\theta})}{\partial \theta_k} \stackrel{!}{=} 0 \quad (k = 1, \ldots, n_{\mathrm{p}}) \tag{7.83}$$

Note that the fact that the first derivatives are zero only assures that an extremal point is obtained. Furthermore, these equations often have several solutions. Therefore, one has to check explicitly which solutions are indeed maxima, and which is the largest one. Note that maximum-likelihood estimators, since they are functions of the samples, are also random variables $\mathrm{ML}_{\theta_k,n}(X_0, \ldots, X_{n-1})$.

As a toy example, we consider the exponential distribution with the pdf given by Eq. (7.39). It has one parameter μ. The log-likelihood function for a sample $\{x_0, x_1, \ldots, x_{n-1}\}$ is in this case

$$\begin{aligned} l(\mu) &= \log \prod_{i=0}^{n-1} f_\mu(x_i) \\ &= \sum_{i=0}^{n-1} \log \left\{ \frac{1}{\mu} \exp\left(-\frac{x_i}{\mu}\right) \right\} \\ &= \sum_{i=0}^{n-1} \left(\log\left\{\frac{1}{\mu}\right\} - \frac{x_i}{\mu} \right) \\ &= n \log\left\{\frac{1}{\mu}\right\} - \frac{n}{\mu}\overline{x} \end{aligned}$$

Taking the derivative with respect to μ we obtain:

$$0 \stackrel{!}{=} \frac{\partial L(\underline{\theta})}{\partial \mu} = n\frac{-1}{\mu^2}\mu - \frac{-n}{\mu^2}\overline{x} = \frac{-n}{\mu^2}(\mu - \overline{x})$$

This implies $\mu = \overline{x}$. It is easy to verify that this corresponds to a maximum. Since the expectation value for the exponential distribution is just $\mathrm{E}[X] = \mu$, this is compatible with the result from Sec. 7.3, where it was shown that the sample mean is an unbiased estimator of the expectation value.

If one applies the maximum-likelihood principle to a Gaussian distribution with parameters μ and σ^2, one obtains (not shown here, see for example

[Dekking et al (2005)]) as maximum-likelihood estimators the sample mean $\overline{x}$ (for μ) and the sample variance s^2 (for σ^2), respectively. This means (see Eq. (7.54)) that the maximum-likelihood estimator for σ^2 is biased. Fortunately, we know that the bias disappears asymptotically for $n \to \infty$. Indeed, it can be shown, under rather mild conditions on the underlying distributions, that all maximum-likelihood estimators $\mathrm{ML}_{\theta_k,n}(X_0, \ldots, X_{n-1})$ for a parameter θ_k are asymptotically unbiased, i.e.

$$\lim_{n\to\infty} \mathrm{E}[\mathrm{ML}_{\theta_k,n}] = \theta_k \tag{7.84}$$

In contrast to the exponential and Gaussian cases, for many applications the maximum-likelihood parameter is not directly related to a standard sample estimator. Furthermore, $\mathrm{ML}_{\theta_k,n}$ can often even not be determined analytically. In this case, one has to optimize the log-likelihood function numerically, for example, using the corresponding methods from the *GNU scientific library* (GSL) (see Sec. 6.3).

GET SOURCE CODE
DIR: `randomness` FILE(S): `max_likely.c`

As example, we consider Fisher-Tippett distribution, see Eq. (7.43), shifted to exhibit the maximum at x_0 instead of at 0. Hence, we have two parameters λ and x_0 to adjust. The function to be optimized (the *target function*), i.e. the log-likelihood function here, must be of a special format when using the minimization functions of the GSL. This first argument of the target function contains the pdf parameters to be adjusted, i.e. the main argument vector of the target function. This argument must be of the type `gsl_vector`, which is a GSL type for vectors. One needs to include `<gsl/gsl_vector.h>` to use this data type. These vectors are created using `gsl_vector_alloc()`, set elements via `gsl_vector_set()`, access elements via `gsl_vector_get()` and delete the vectors via `gsl_vector_free()`. The usage of these functions should be self-explanatory from the examples below, but you may also have a look at the GSL documentation [Galassi et al. (2006)].

The second argument of the target function contains *one* pointer to all additional data needed to calculate the target function, i.e. the sample in this case. Thus, the sample must be stored in *one* chunk of memory. For this purpose, we use the following structure type:

```
typedef struct
{
  int       n;       /* number of sample points; */
  double   *x;                          /* sample */
}
sample_t;
```

Since the GSL package contains actually minimization functions, while we are interested in a maximum, the actual log-likelihood function returns minus the log-likelihood. The log-likelihood function reads as follows:

```
1  double ll_ft(const gsl_vector *par, void *param)
2  {
3    double lambda, x0;                    /* parameters of pdf */
4    sample_t *sample;                              /* sample */
5    double sum;          /* sum of log-likelihood contributions */
6    int i;                                  /* loop counter */
7
8    lambda = gsl_vector_get(par, 0);               /* get data */
9    x0 = gsl_vector_get(par, 1);
10   sample = (sample_t *) param;
11
12   sum = sample->n*log(lambda);    /* calculate log likelihood */
13   for(i=0; i<sample->n; i++)
14     sum -= lambda*(sample->x[i]-x0) +
15            exp(-lambda*(sample->x[i]-x0));
16
17   return(-sum);                    /* return - log likelihood */
18 }
```

First, we convert the pointers passed as arguments to the data format that we find useful (lines 8–10). Next, the actual log likelihood

$$l(\lambda, x_o) = n \log \lambda - \lambda \sum_{i=0}^{n-1} (x_i - x_0) - \sum_{i=0}^{n-1} \exp(-\lambda(x_i - x_0))$$

is calculated in lines 12–15 and finally returned with inverted sign (line 17).

The GSL has built in several minimization algorithms. They are all put under one of two frameworks. One framework is for algorithms which require the target function and its first derivatives. The other framwork contains algorithms where just the target function is sufficient. Here we use the *simplex algorithm*, which belongs to the latter form. It works by spanning a simplex,[16] evaluating the target functions at the corners of the simplex, and iteratively changing the simplex until it is very small and contains the solution. Note that the algorithm is only able to find local minima, and only one of them. If several minima exist, the choice of the initial parameters strongly influence the final results; Here, one maybe has to try several parameters. For details see [Galassi et al. (2006)]. Here we only show how to use the minimizer. The minimizer itself is stored in a special data structure of type `gsl_multimin_fminimizer`. The target function has to be put into a "surrounding" variable of type `gsl_multimin_function`. Furthermore, one needs two `gsl_vector` variables to store the current estimate for the optimum (specifying the position of the simplex) and to store the size of the simplex. Also, `par` is used here to state the dimension of the target function argument (2) and `sample` to store the sample.

These variables are declared as follows:

[16] A simplex is a convex set in an n-dimensional space generated by $n + 1$ corner points.

```
int num_par;                          /* number of parameters */
sample_t sample;                                  /* sample */

gsl_multimin_fminimizer *s;           /* the full mimimizer */
gsl_vector *simplex_size;        /* (relative) simplex size */
gsl_vector *par; /* params to be optimized = args of target */
gsl_multimin_function f;  /* holds function to be optimized */
```

The actual allocation and initialization of these variables may look as follows:

```
sample.n = 10000;                           /* initilization */
sample.x = (double *) malloc(sample.n*sizeof(double));
num_par = 2;

f.f = &ll_ft;                     /* initialize minimization */
f.n = num_par;
f.params = &sample;
simplex_size = gsl_vector_alloc(num_par);  /* alloc simplex */
gsl_vector_set_all(simplex_size, 1.0);      /* init simplex */
par = gsl_vector_alloc(num_par);  /* alloc + init arguments */
gsl_vector_set(par, 0, 1.0);
gsl_vector_set(par, 1, 1.0);
s =
  gsl_multimin_fminimizer_alloc(gsl_multimin_fminimizer_nmsimplex,
                                num_par);
gsl_multimin_fminimizer_set(s, &f, par, simplex_size);
```

The set-up of the minimizer object comes in two steps, first allocation using `gsl_multimin_fminimizer_alloc()`, then initialization via `gsl_multimin_fminimizer_set()` while passing the target function, the starting point `par` and the (initial) simplex size.[17] The `sample.x[]` array has to be filled with the actual sample (not shown here).

The minimization loop looks as follows:

```
do                                    /* perform minimization */
{
  iter++;
  status = gsl_multimin_fminimizer_iterate(s);  /* one step */
  if(status)    /* error ? */
    break;
  size = gsl_multimin_fminimizer_size(s);    /* converged ? */
  status = gsl_multimin_test_size(size, 1e-4);
}
while( (status == GSL_CONTINUE) && (iter<100) );
```

The main work is done in `gsl_multimin_fminimizer_iterate()`. Then it is checked whether an error has occurred. Next, the size of the simplex is calculated and finally tested whether the size falls below some limit, 10^{-4} here.

[17] The simplex is spanned by `par` and the n vectors given by `par` plus $(0, \ldots, 0,$ `simplex_size[i]`$, 0, \ldots, 0)$ for $i = 1, \ldots, n$.

The actual estimate of the parameters can be obtained via `gsl_vector_get(s->x, 0)` and `gsl_vector_get(s->x, 1)`. Note that finally all allocated memory should be freed:

```
gsl_vector_free(par);                    /* free everything */
gsl_vector_free(simplex_size);
gsl_multimin_fminimizer_free(s);
free(sample.x);
```

As an example, $n = 10000$ data points were generated according to a Fisher-Tippett distribution with parameters $\lambda = 3.0$, $x_0 = 2.0$. With the above starting parameters, the minimization converged to the values $\hat{\lambda} = 2.995$ and $\hat{x}_0 = 2.003$ after 39 iterations.

7.6.2 Data fitting

In the previous section, the parameters of a probability distribution are chosen such that the distribution describes the data best. Here, we consider a more general case, called *modeling of data*. As explained above, here a sample of triplets $\{(x_0, y_0, \sigma_0), (x_1, y_1, \sigma_1), \ldots, (x_{n-1}, y_{n-1}, \sigma_{n-1})\}$ is given. Typically, the y_i are measured values obtained from a simulation with some control parameter (e.g. the temperature) fixed at different values x_i; σ_i is the corresponding error bar of y_i. Here, one wants to determine parameters $\underline{\theta} = (\theta_1, \ldots, \theta_{n_\mathrm{p}})$ such that the given parametrized function $y_{\underline{\theta}}(x)$ fits the data "best", one says one wants to *fit* the function to the data. Similar to the case of fitting a pmf or a pdf, there is no general principle of what "best" means.

Let us assume that the y_i are random variables, i.e. comparing different simulations. Thus, the measured values are scattered around their "true" values $y_{\underline{\theta}}(x_i)$. This scattering can be described approximately by a Gaussian distribution with mean $y_{\underline{\theta}}(x_i)$ and variance σ_i^2:

$$q_{\underline{\theta}}(y_i) \sim \exp\left(-\frac{(y_i - y_{\underline{\theta}}(x_i))^2}{2\sigma_i^2}\right) . \tag{7.85}$$

This assumption is often valid, e.g. when each sample point y_i is itself a sample mean obtained from a simulation performed at control parameter value x_i, and σ_i is the corresponding error bar. The log-likelihood function for the full data sample is

$$\begin{aligned} l(\underline{\theta}) &= \log \prod_{i=0}^{n-1} q_{\underline{\theta}}(y_i) \\ &\sim -\sum_{i=0}^{n-1} \frac{1}{2} \left(\frac{y_i - y_{\underline{\theta}}(x_i)}{\sigma_i}\right)^2 \end{aligned}$$

Maximizing $l(\underline{\theta})$ is equivalent to minimizing $-2l(\underline{\theta})$, hence one minimizes the *mean-squared difference*

$$\chi^2_{\underline{\theta}} = \sum_{i=0}^{n-1} \left(\frac{y_i - y_{\underline{\theta}}(x_i)}{\sigma_i} \right)^2 \tag{7.86}$$

This means the parameters $\underline{\theta}$ are determined such that function $y_{\underline{\theta}}(x)$ follows the data points $\{(x_0, y_0), \ldots (x_{n-1}, y_{n-1})\}$ as close as possible, where the deviations are measured in terms of the error bars σ_i. Hence, data points with smaller error bar enter with more *weight*. The full procedure is called *least-squares fitting*.

The minimized mean-squared difference is a random variable. Note that the different terms are not statistically independent, since they are related by the n_p parameters $\hat{\underline{\theta}}$ which are determined via minimizing $\chi^2_{\underline{\theta}}$. As a consequence, the distribution of $\chi^2_{\hat{\underline{\theta}}}$ is approximately given by chi-squared distribution (see Eq. (7.45) for the pdf) with $n - n_\mathrm{p}$ degrees of freedom. This distribution can be used to evaluate the statistical significance of a least-squares fit, see below.

In case, one wants to model the underlying distribution function for a sample as in Sec. 7.6.1, say for a continuous distribution, it is possible in principle to use the least-squares approach as well. In this case one would fit the parametrized pdf to a histogram pdf, which has also the above mentioned sample format $\{(x_i, y_i, \sigma_i)\}$. Nevertheless, although the least-squares principle is derived using the maximum-likelihood principle, usually different parameters are obtained if one fits a pdf to a histogram pdf compared to obtaining these parameters from a direct maximum-likelihood approach. Often [Bauke (2007)], the maximum-likelihood method gives more accurate results. Therefore, one should use a least-squares fit mainly for a fit of a non-pmf/non-pdf function to a data set.

Fortunately, to actually perform least-squares fitting, you do not have to write your own fitting functions, because there are very good fitting implementations readily available. Both programs presented in Sec. 7.4, *gnuplot* and *xmgrace*, offer fitting to arbitrary functions. It is advisable to use *gnuplot*, since it offers higher flexibility for that purpose and gives you more information useful to estimate the quality of a fit.

As an example, let us suppose that you want to fit an algebraic function of the form $f(L) = e_\infty + aL^b$ to the data set of the file `sg_e0_L.dat` shown on page 42. First, you have to define the function and supply some rough (non-zero) estimations for the unknown parameters. Note that the exponential operator is denoted by `**` and the standard argument for a function definition is `x`, but this depends only on your choice:

```
gnuplot> f(x)=e+a*x**b
gnuplot> e=-1.8
gnuplot> a=1
gnuplot> b=-1
```

The actual fit is performed via the `fit` command. The program uses the non-linear least-squares Levenberg-Marquardt algorithm [Press et al. (1995)], which

allows a fit data to almost all arbitrary functions. To issue the command, you have to state the fit function, the data set and the parameters which are to be adjusted. First, we consider the case where just two columns of the data are used or available (in this case, *gnuplot* assumes $\sigma_i = 1$). For our example you enter:

```
gnuplot> fit f(x) "sg_e0_L.dat" via e,a,b
```

Then *gnuplot* writes log information to the output describing the fitting process. After the fit has converged it prints for the given example:

```
After 17 iterations the fit converged.
final sum of squares of residuals : 7.55104e-06
rel. change during last iteration : -2.42172e-09

degrees of freedom (ndf) : 5
rms of residuals      (stdfit) = sqrt(WSSR/ndf)      : 0.00122891
variance of residuals (reduced chisquare) = WSSR/ndf : 1.51021e-06

Final set of parameters            Asymptotic Standard Error
=======================            ==========================

e               = -1.78786         +/- 0.0008548    (0.04781%)
a               = 2.5425           +/- 0.2282       (8.976%)
b               = -2.80103         +/- 0.08265      (2.951%)


correlation matrix of the fit parameters:

               e      a      b
e               1.000
a               0.708  1.000
b              -0.766 -0.991  1.000
```

The most interesting lines are those where the results $\underline{\hat{\theta}}$ for your parameters along with the standard error bar are printed.[18] Additionally, the quality of the fit can be estimated by the information provided in the three lines beginning with "`degree of freedom`". The first of these lines states the number of degrees of freedom, which is just $n - n_{\rm p}$. The mean-squared difference $\chi^2_{\underline{\hat{\theta}}}$ is denoted as `WSSR` in the *gnuplot* output. A measure of quality of the fit is the probability Q that the value of the mean-squared difference is equal or larger compared to the value from the current fit, given the assumption that the data points are distributed as in Eq. (7.85) [Press et al. (1995)]. The larger the value of Q, the better is the quality of the fit. As mentioned above, Q can be evaluated from a chi-squared distribution with $n - n_{\rm p}$ degrees of freedom. To calculate Q using the *gnuplot output* you can use the little program `Q.c`

[18] These "error bars" are calculated in a way which is in fact correct only when fitting linear functions; hence, they have to be taken with care.

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <gsl/gsl_cdf.h>

int main(int argc, char *argv[])
{
  double WSSRndf;
  int ndf;

  if(argc != 3)
  {
    printf("USAGE %s <ndf> <WSSR/ndf>\n", argv[0]);
    exit(1);
  }
  ndf = atoi(argv[1]);
  sscanf(argv[2], "%lf", &WSSRndf);
  printf("# Q=%e\n", gsl_cdf_chisq_Q(ndf*WSSRndf, ndf));

  return(0);
}
```

which uses the `gsl_cdf_chisq_Q()` function from the GSL (see Sec. 6.3). The program is called in the form `Q <ndf> <WSSR/ndf>`, which can be taken from the *gnuplot* output. Note that in this case we obtain $Q = 1$, which is so large, because $\sigma_i = 1$ was used, see below.

To watch the result of the fit along with the original data, just enter

```
gnuplot> plot "sg_e0_L.dat" w e, f(x)
```

The result is displayed in Fig. 7.29. Please note that the convergence depends on the initial choice of the parameters. The algorithm may be trapped into a local minimum in case the parameters are too far away from the best values. Try the initial values `e=1`, `a=-3` and `b=1`! Furthermore, not all function parameters have to be subjected to the fitting. Alternatively, you can set some parameters to fixed values and omit them from the `via` list at the end of the `fit` command. Remember that in the above example all data points enter into the result with the same weight, i.e. $\sigma_i = 1\,\forall i$ is assumed. You can tell the algorithm to consider the error bars, for example supplied in the third column, by typing

```
gnuplot> fit f(x) "sg_e0_L.dat" using 1:2:3 via e,a,b
```

Then, data points with larger error bars have less influence on the results. In this case a different result whith smaller value of Q will arise (try it !).

Finally, you can also restrict the data points which are considered for the fit, which is applicable if only a subset of the sample follows the function law you are considering. This can be done in the same way as restricting the range of plotted values, for instance using

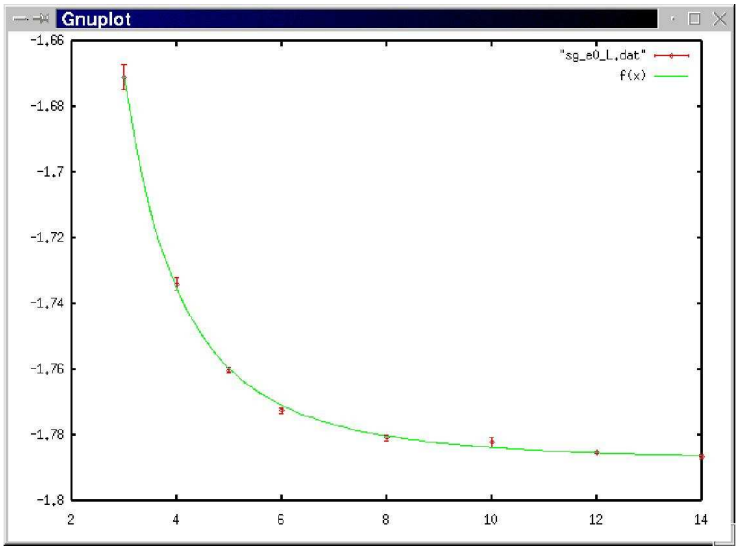


Figure 7.29: *Gnuplot* window showing the result of a fit command along with the input data.

```
gnuplot> fit [5:12] f(x) "sg_e0_L.dat" using 1:2:3 via e,a,b
```

More information on how to use the `fit` command, such as fitting higher-dimensional data, can be obtained when using the *gnuplot* online help via entering `help fit`.

Exercises

(solutions: see CD enclosed with book)

1. **Sampling from discrete distribution**

   Design, implement and test a function, which returns a random number which is distributed according to some discrete distribution function stored in an array `F`, as describe in Sec. 7.2.2. The function prototype reads as follows:

SOLUTION SOURCE CODE
DIR: `randomness` FILE(S): `poisson.c`

```
/******************* rand_discrete() ****************/
/** Returns natural random number distributed        **/
/** according a discrete distribution given by the   **/
/** distribution function in array 'F'               **/
/** Uses search in array to generate number          **/
/** PARAMETERS: (*)= return-paramter                 **/
/**       n: number of entries in array              **/
/**       F: array with distribution function        **/
/** RETURNS:                                         **/
/**     random number                                **/
/*****************************************************/
int rand_discrete(int n, double *F)
```

   For simplicity, you can use the `drand48()` function from the standard C library to generate random numbers distributed according to $U(0, 1)$.

   Furthermore, design, implement and test a function, which allocates and initializes the array `F` for a Poisson distribution with parameter μ, see Eq. (7.27) for the probability mass function. The function should determine automatically how many entries of `F` are needed, depending on the paramater μ. The function prototype reads as follows:

```
/******************** init_poisson() ****************/
/** Generates  array with distribution function      **/
/** for Poisson distribution with mean mu:           **/
/** p(k)=mu^k*exp(-mu)/x!                            **/
/** The size of the array is automatically adjusted. **/
/** PARAMETERS: (*)= return-paramter                 **/
/**   (*) n_p: p. to number of entries in table      **/
/**        mu: parameter of distribution             **/
/** RETURNS:                                         **/
/**     pointer to array with distribution function  **/
/*****************************************************/
double *init_poisson(int *n_p, double mu)
```

   Hints: To determine the array sizes, you can first loop over the probabilities and take the first value `k_0` where $p($`k_0`$) = 0$ within the precision of the numerics. This value of `k_0` serves as array size. Alternatively, you start with some size and extend the array if needed by doubling its size. For testing purposes, you can generate many numbers, calculate the mean and compare it with μ. Alternatively, you could record a histogram (see Chap. 3) and compare with Eq. (7.27).

2. **Inversion Method for Fisher-Tippett distribution**

SOLUTION SOURCE CODE
DIR: `randomness` FILE(S): `fischer_tippett.c`

Design, implement and test a function, which returns a random number which is distributed according to the Fisher-Tippett distribution Eq. (7.43) with parameter λ. Use the inversion method.
The function prototype reads as follows:

```
/******************** rand_fisher_tippett() ***********/
/** Returns random number which is distributed       **/
/** according the Fisher-Tippett distribution        **/
/** PARAMETERS: (*)= return-paramter                 **/
/**       lambda: parameter of distribution          **/
/** RETURNS:                                         **/
/**     random number                                **/
/*****************************************************/
double rand_fisher_tippett(double lambda)
```

Remarks: For simplicity, you can use the `drand48()` function from the standard C library to generate random numbers distributed according to $U(0,1)$. To test your function, you can calculate the mean of the generated numbers, for instance, and compare it with the expectation value $\sim 0.57721/\lambda$.

3. **Variance of data sample**

SOLUTION SOURCE CODE
DIR: `randomness` FILE(S): `variance.c`

Design, implement and test a function, which calculates the variance s^2 of a sample of data points. Use directly Eq. (7.51), i.e. do *not* use an equivalent form of Eq. (7.21), since this form is more susceptible to rounding errors.
The function prototype reads as follows:

```
/********************** variance() *******************/
/** Calculates the variance of n data points        **/
/** PARAMETERS: (*)= return-paramter                 **/
/**        n: number of data points                  **/
/**        x: array with data                        **/
/** RETURNS:                                         **/
/**     variance                                     **/
/*****************************************************/
double variance(int n, double *x)
```

Remark: The so-called corrected double-pass algorithm [Chan et al. (1983)] aims at further reducing the rounding error. It is based on the equation

$$s^2 = \frac{1}{n}\left[\sum_{i=0}^{n-1}(x-\overline{x})^2 - \frac{1}{n}\left(\sum_{i=0}^{n-1}(x_i-\overline{x})\right)^2\right] .$$

The second would be zero for exact arithmetic and accounts for rounding erros occurring in the second term. It becomes important in particular if the expectation value is large. Perform experiments for generating Gaussian distributed number with $\sigma^2 = 1$ and $\mu = 10^{14}$, without and with the correction.

4. **Bootstrap**

   Design, implement and test a function, which uses bootstrapping to calculate the confidence interval at significance level α given in Eq. (7.66).

SOLUTION SOURCE CODE
DIR: `randomness` FILE(S): `bootstrap_ci.c`

   The function prototype reads as follows:

```
/***************** bootstrap_ci() *********************/
/** Calculates a confidence interval by 'n_resample' **/
/** times resampling the given sample points         **/
/** and each time evaluation the estimator 'f'       **/
/** PARAMETERS: (*)= return-paramter                 **/
/**           n: number of data points               **/
/**           x: array with data                     **/
/**  n_resample: number of bootstrap iterations      **/
/**       alpha: confidence level                    **/
/**           f: function (pointer) = estimator      **/
/**     (*) low: (p. to) lower boundary of conf. int.**/
/**    (*) high: (p. to) upper boundary of conf. int.**/
/** RETURNS:                                         **/
/**     (nothing)                                    **/
/****************************************************/
void bootstrap_ci(int n, double *x, int n_resample,
                  double alpha, double (*f)(int, double *),
                  double *low, double *high)
```

   Hints: Use the function `bootstrap_variance()` as example. To get the entries at the positions defined via Eq. (7.66), you can sort the bootstrap sample first using `qsort()`, see Sec. 6.1.

   You can test your function by using the provided main file `bootstrap_test.c`, the auxiliary files `mean.c` and `variance.c` and by compiling with `cc -o bt bootstrap_test.c bootstrap_ci.c mean.c -lm -DSOLUTION`. Note that the macro definition `-DSOLUTION` makes the `main()` function to call `bootstrap_ci()` instead of `bootstrap_variance()`.

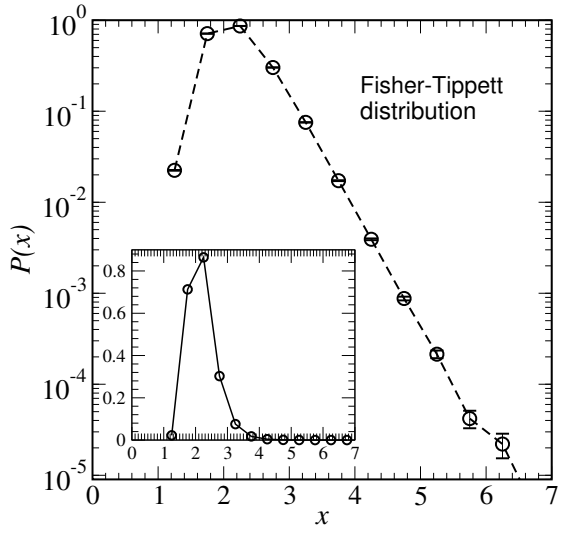
5. **Plotting data**

   Plot the data file `FTpdf.dat` using *xmgrace*. The file contains a histogram pdf generated for the Fisher-Tippett distribution. The file format is 1st column: bin number, 2nd: bin midpoint, 3rd: pdf value, 4th: error bar. Use

SOLUTION SOURCE CODE
DIR: `randomness` FILE(S): `FTplot.agr`

   the "block data" format to read the files (columns 2,3,4). Create a plot with inset. The main plot should show the histogram pdf with error bars and logarithmically scaled y axis, the inset should show the data with linear axes. Describe the plot using a text label placed in the plot. Choose label sizes, line width and other styles suitably. Store the result as `.agr` file and export it to a postscript (eps) file.

   The result should look similar to:



6. **Chi-squared test**

SOLUTION SOURCE CODE
DIR: `randomness`
FILE(S): `chi2hh.c`

Design, implement and test a function, which calculates the χ^2 test statistics for two histograms $\{h_i\}, \{\hat{h}_i\}$ according Eq. (7.69). The function should return the p-value, i.e. the cumulative probability ("p-value") that a value of χ^2 or larger is obtained under the assumption that the two histograms were obtained by sampling from the same (discrete) random variable.

The function prototype reads as follows:

```
/******************** chi2_hh() ***********************/
/** For chi^2 test: comparison of two histograms      **/
/** to probabilities: Probability to                  **/
/** obtain the corresponding  chi2 value or worse.    **/
/** It is assumed that the total number of data points**/
/** in the two histograms is equal !                  **/
/**                                                   **/
/** Parameters: (*) = return parameter                **/
/**  n_bins: number of bins                           **/
/**       h: array of histogram values                **/
/**      h2: 2nd array of histogram values            **/
/**                                                   **/
/** Returns:                                          **/
/**       p-value                                     **/
/*******************************************************/
double chi2_hh(int n_bins, int *h, int *h2)
```

Hints: Use the functio `chi2_hd()` as example. Include a test, which verifies that the total number of counts in the two histograms agree.

To test the function: Generate two histograms according to a binomial distribution with parameters $n =$ `par_n`$= 10$ and $p = 0.5$ or $p =$ `par_p`. Perform a

loop for different values of `par_p` and calculate the p-value each time using the `gsl_cdf_chisq_Q()` function of the *GNU scientific library* (GSL) (see Sec. 6.3).

7. **Linear correlation coefficient**

SOLUTION SOURCE CODE
DIR: `randomness` FILE(S): `lcc.c`

Design, implement and test a function, which calculates the linear correlation coefficient r to measure the strength of a correlation for a sample $\{(x_0, y_0), (x_1, y_1), \ldots, (x_{n-1}, y_{n-1})\}$.
The function prototype reads as follows:

```
/*************************** lcc() ********************/
/** Calculates the linear correlation coefficient     **/
/**                                                   **/
/** Parameters: (*) = return parameter                **/
/**     n: number of data points                      **/
/**     x: first element of sample set                **/
/**     y: second element of sample set               **/
/**                                                   **/
/** Returns:                                          **/
/**       r                                           **/
/*******************************************************/
double lcc(int n, double *x, double *y)
```

Remark: Write a `main()` function which generates a sample in the following way: the x_i numbers are generated from a standard Gaussian distribution $N(0, 1)$ while each y_i number is drawn from a Gaussian distribution with expectation value κx_i (variance 1). Study the result for different values of κ and n.

8. **Least-squares fitting**

SOLUTION SOURCE CODE
DIR: `randomness` FILE(S): `fitFT.gp` `fisher_tippett2.c`

Copy the program from exercise (2) to a new program and change it such that numbers for a shifted Fisher-Tippett with parameters λ and peak position x_0 are generated. The numbers should be stored in a histogram and a histogram pdf should be written to the standard output.

- Choose the histogram parameters (range, bin range) such that the histograms match the generated data well.
- Run the program to generate $n = 10^5$ numbers for parameters $x_0 = 2.0$ and $\lambda = 3.0$. Pipe the histogram pdf to a file (e.g. using `> ft.dat` at the end of the call).
- Plot the result using *gnuplot*.
- Define the pdf for the Fisher-Tippett distribution in *gnuplot* and fit the function to the data with x_0 and λ as adjustable parameters. Choose a suitable range for the fit.
- Plot the data together with the fitted function.
- How does the result compare to the maximum-likelihood fit presented in Sec. 7.6.1?
- Does the fit (in particular for λ) get better if you increase the number of sample points to 10^6?

Hints: The shift is implemented by just adding x_0 to the generated random number. Use either the histograms from Chap. 3, or implement a "poor-mans histogram" via an array `hist` (see also in the `main()` function of the `reject.c` program partly presented in Sec. 7.2.4).

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